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(NASA-CR-167990-Vol-2) ANALYTICAL MCDELING OF OFERATING CHARACTERISTICS OF FROMIXING-FEDVAPORIZING FORI-ATE MIXING PASSAGES. VOLUME 2: USER'S MANUAL (United Technologies Research Center) 158 r

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NASA CR-167990 R82-915362-40

Analytical Modeling of Operating Characteristics of Premixing-Prevaporizing Fuel-Air Mixing Passages

Vol. II User's Manual

Olof L. Anderson Louis M. Chiappetta David E. Edwards John B. McVey



February 1982

Prepared for NASA Lewis Research Center Under Contract NAS3-21269

1. Report No.	2. Government Access	ion No.	3. Recipient's Catalog	No.
4. Title and Subtitle	L		5. Report Date	
Analytical Modeling of Operat	ing Characteris	stice of	February 1982	?
Premixing-Prevaporizing Fuel-		1	6. Performing Organia	zation Code
7. Author(s) O. L. Anderson, L. M	. Chiappetta		8. Performing Organiz R82-915362-40	
D. E. Edwards, J. B.		Ĺ	K02-913302-40)
			10. Work Unit No.	
9. Performing Organization Name and Address United Technologies Research	Center	Ĺ		
Silver Lane	Center		11. Contract or Grant	No.
East Hartford, CT 06108			NAS3-21269	
East Hartiord, CI 00108			13. Type of Report ar	nd Period Covered
12. Sponsoring Agency Name and Address			Final Report	(Volume I)
NASA Lewis Research Center			.User's Manual	
21000 Brookpark Road		i	14. Sponsoring Agency	Code
Cleveland, OH 44135				
15. Supplementary Notes				
NACA Project Manager - C I	Mamale			
NASA Project Manager - C. J.				
UTRC Project Manager - O. L.	Anderson			
16. Abstract A model for predicting the di	stribution of 1	iouid fuel drople	ate and fuel v	anor in pre-
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vicinity of the fuel droplets				
The model, as represented by				
air mixing passage designs ar	nd the results	are discussed. A	n application	of the
autoignition model is also pr	esented.			
17. Key Words (Suggested by Author(s))		18. Distribution Statement		
Premixing-Prevaporizing Passa	iges			
Autoignition Model				
Two-phase Flow				
Two- and Three-Dimensional Fl Computer Program	ow Models			
10 Committee Classif (of this report)	20 Security Classif (of this page)	21. No. of Pages	22 Price*

Unclassified

103

Unclassified

^{*} For sale by the National Technical Information Service, Springfield, Virginia 22151

Analytical Modeling of Operating Characteristics of Premixing-Prevaporizing Fuel-Air Mixing Passages

Volume II - User's Manual

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1.0 SUMMARY

A User's Manual describing the operation of three computer codes (ADD code, PTRAK code, and VAPDIF code) is presented herein. This manual is organized for the convenience of the user and contains sections describing the general features of the computer codes, the input/output formats, run streams, and sample input cases. It is presented in loose leaf format so that changes may be made easily as additional capabilities are added to the computer programs.

This User's Manual constitutes Volume II of the final report under NASA Contract NAS3-21269.

2.0 INTRODUCTION

This User's Manual describes the computer codes used to calculate the operating characteristics of premixing-prevaporizing fuel/air mixing passages. The calculation procedure utilizes three computer codes: the ADD code which calculates the axisymmetric or two-dimensional distributions of velocity, pressure, and temperature of the air flow; the PTRAK code which calculates the nonequilibrium heat-up, vaporization, and trajectories of the liquid fuel droplets in a three-dimensional flow field; and the VAPDIF code which calculates the diffusion of fuel vapor or critical autoignition species into a moving air stream. A detailed description of the analytical models and numerical procedures used in these computer codes is given in Volume I. The User's Manual, Volume, II, contains a description of the operation of the computer codes.

The ADD code was originally developed for NASA Lewis Research Center under Contract NAS3-15402 (Ref. 1). Important revisions, including the conformal mapping coordinate generator, were developed for the U. S. Army Air Mobility Research and Development Laboratory under Contract No. DAAJ02-73-C-0037 (Ref. 2). Further development and improvements to the ADD code were funded by United Technologies Research Center and Pratt & Whitney Aircraft, Commercial Products Division. Additional improvements, including the incorporation of a two-equation model of turbulence into the ADD code, was sponsored by NASA Lewis Research Center under Contract NAS3-21853 (Ref. 3). A complete description of the ADD code is given in Ref. 4 together with a new coordinate generator sponsored under contract DEN3-235.

The original version of the PTRAK code was developed by United Technologies Research Center with its own funding. This version was based on a simple equilibrium vaporization model for single-component fuels. The nonequilibrium heat-up and vaporization model for a distillate fuel was developed under the current contract, NAS3-21269.

The VAPDIF code was developed exclusively under the current contract although it is largely based on the Contractor's experience in developing three-dimensional parabolic forward marching computer codes for predicting the behavior of compressible flows.

This User's Manual is organized into several sections for the convenience of the computer code user. Section 3.0 contains a description of the general features of each of the computer codes to provide the user with an overview of the types of problems which can be solved. Sections 4.0, 5.0 and 6.0 contain descriptions of the operation of each of the computer codes. Sections 3.0 through 6.0 should provide the user with sufficient information of setup and solve typical problems within the scope of the computer codes. Sections 7.0, 8.0, 9.0 present a more detailed description of the PTRAK and VAPDIF codes. A description of the ADD code is given in Ref. 4.

This User's Manual constitutes Volume II of the final report under Contract NAS3-21269.

3.0 GENERAL FEATURES

3.1 General Features of ADD Code

Program Language

The Annular Diffuser Deck (ADD) code source program is written in FORTRAN V computer language for use on a UNIVAC 1100/81A computer. Some machine specific language, such as PARAMETER and INCLUDE FØRTRAN statements, is used. However, these statements may be replaced easily by equivalent code for use on other machines. Successful conversions of the code to both IBM and CDC computers have been made and these versions of the code are available. The ADD code makes use of a UNIVAC routine NTRAN which stores and retrieves large data blocks on disc files; however, the ADD code is organized so that NTRAN is easily replaced by the equivalent FØRTRAN DEFINE FILE. Finally, it should be noted that the ADD code makes use of least squares spline fitting and smoothing subroutines provided by IMSL, Inc. which are available at all major computer centers.

Fluid Properties

The ADD code can treat any compressible fluid with constant thermodynamic properties for the gas constant R and the specific heats Cp and Cv. The molecular viscosity, which is temperature dependent, is estimated using Sutherland's law; the molecular thermal conductivity is calculated using a constant value for Prandtl number. The viscosity of the fluid at standard conditions and Prandtl number are input parameters. If these properties are not specified in the input data, the ADD code uses the properties of air at standard conditions.

Types of Flow That May Be Treated

The ADD code may be used to treat subsonic compressible laminar or turbulent swirling flow in axisymmetric ducts or nonswirling flow in two-dimensional ducts. The duct may be annular or two-dimensional with both inner and outer walls; or, it may be an axisymmetric duct with only an outer wall. Subsonic flows have been treated successfully up to the sonic line. The mixing of hot and cold streams has also been analyzed using the ADD code. The code is not applicable to flows containing regions of separation or reverse flow.

Duct Geometry Option (IMPT3)

The flow through axisymmetric or two-dimensional ducts may be calculated provided that the principal flow direction is axial; however, the duct cannot contain a right-angle turn. The ADD code is not applicable to flows in ducts with discontinuities in flow area that produce regions of flow separation.

For convenience, provision is made in the code to analyze flows in straight annular ducts (IØPT3=1) or in straight wall, annular diffusers (IØPT3=3) using only a few input parameters. For ducts of arbitrary shape (IØPT3=2), the coordinates (radii) of the inner and outer walls are specified at JLPTS equally-spaced axial stations. To assure that the curve representing the duct contour has continuous first and second derivatives, a least-squares spline fitting, smoothing and interpolation procedure is included in the code. This procedure is used wherever the number of streamwise stations (JL) is not equal to JLPTS.

The specification of the duct geometry must include a straight, annular inlet section whose length is at least equal to its height. Two-dimensional ducts are treated as annular ducts in which the height of the duct is small compared to the radius of the duct. Numerical experiments have shown that, if the height of the duct is less than 1/100 of the duct radius, the flow is essentially two-dimensional to an accuracy of three decimal places.

Inlet Flow Options (IØPT1)

Any arbitrary inlet flow conditions may be specified which are consistent with the equations of motion and the turbulence model. Two types of input data are required: (1) specification of the inviscid free stream and core flow conditions, and (2) specification of the laminar or turbulent boundary layer flow parameters. With IOPT1=3, 4, 9, the flow is assumed to be turbulent and with IOPT1=7, 8, the flow is assumed to be laminar. With IOPT1= 3 or 7, the core flow is calculated assuming that the stagnation pressure and stagnation temperature are constant across the duct. The input Mach number and swirl angle determine the velocities and weight flow, and the static pressure is determined by solving the conservation equation for radial momentum. When IOPTl= 4 or 8, the inlet core flow is determined by specifying KLL data points for fractional distance Y, stagnation pressure $P_{T}(Y)$, static pressure P(Y), swirl angle $\alpha(Y)$, and stagnation temperature $T_T(Y)$. For IOPT1=9, the core flow is determined by specifying KLL data points for fractional distance Y, streamwise velocity $U_S(Y)$, stagnation pressure $P_T(Y)$, swirl velocity $U_{\underline{\varphi}}(Y)$, and stagnation temperature $T_{\underline{T}}(Y)$. Isentropic flow relations and radial momentum conservation equations are used to determine the remaining variables. In addition, when IOPTI=4, 8 or 9, the corresponding exit flow data must be provided. These data are not required by the calculation procedure but are used only by plotting routines which can be used to compare calculated and measured exit flow profiles. If the exit plane data are not available, the inlet plane data may be repeated.

The boundary layer velocity and temperature profiles are constructed from known analytic solutions using the boundary layer displacement thickness (δ^*) and a power law (1/n) velocity profile. For laminar boundary layers (IOPT1=7, 8) a Blasius profile is assumed. For turbulent flows (IOPT1=3, 4, 9), Cole's boundary layer profile is used with the shape parameter determined from 1/n.

In many flow situations, it is often more convenient to specify the weight flow rather than velocity or Mach number. For these situations, the user may specify the weight flow when using $I\emptyset PTl=4$ or 8. The static pressure profile is automatically adjusted to obtain the required weight flow with the other input variables held fixed.

It should be noted that the initial plane conditions must satisfy the laws of motion and be compatible with the turbulence model. Therefore, the ADD code makes many checks on the input data to assure satisfactory starting conditions. As an example, the initial plane data are checked to determine if the radial momentum conservation equation is satisfied. If it is not satisfied, the input static pressure profile is replaced by the static pressure profile calculated from the radial momentum equation and a DIAGNØSTIC message is printed. The weight flow calculated from the initial plane data is checked to see if it is greater than the choked-flow value. If it is greater, the calculation stops and the value of the choked weight flow is printed out. Checks are made to assure that the boundary layer profile can be matched to the free stream core flow; the necessary adjustments are made automatically and the calculation continues. In all cases where adjustments to the input data are made and the calculation continues, a DIAGNØSTIC message is printed. When no adjustment is possible or when the flow situation is physically impossible, the calculation stops and the user is notified with a DIAGNØSTIC mossage. A list of these DIAGNØSTIC messages is given in Section 4.4

Grid Selection

The user may determine the calculation grid using input parameters or the grid may be determined automatically. In either case the user must specify the number of streamwise stations (JL) and the number of streamlines (KL). Experience has shown that a 50 x 50 mesh is suitable for most problems. Default options exist for both the distribution of mesh points in the cross flow direction as specified by the mesh distortion parameters DDS and the streamwise step size parameter KDS. In selecting the mesh distortion parameters DDS, numerical accuracy requires that a sufficient number of mesh points exist in the turbulent sublayer. In practice, the first mesh point from the wall should be at $Y^+ = 1.0$ and at least 20 mesh points should be in the boundary layer. These criteria depend on both the flow Reynolds number and wall friction coefficient. Therefore, if DDS is not specified in the input data, a value for DDS is calculated using an algorithm which produces good results for most cases. The value for the streamwise step size parameter KDS depends on the boundary layer thickness and rate of growth of the boundary layer. If KDS is not specified, the code selects a value for KDS between each streamwise station using an algorithm which produces satisfactorily results for most cases.

Print Options (IØPT4)

The frequency and quantity of output are controlled by the print option IPT4. If IOPT4 > 0, the output consists of the mean flow variables including streamwise

velocity U_8 , tangential velocity U_{φ} , static pressure P, stagnation pressure P_T , stagnation temperature T_T , and Mach number M at each streamwise station for JL stations; this printout occurs at every IØPT4th station. If 10PT4 \leq -1, additional information is printed including the effective turbulent viscosity and thermal conductivity, the boundary layer solution in universal coordinates $U^+(Y^+)$, and the turbulent kinetic energy distribution; this information is printed every IØPT4th station.

Diagnostics

The ADD code makes numerous checks during the progress of the calculation. If the program is able to remedy a detected problem, a DIAGNØSTIC is printed and the calculation continues. If a fatal error is detected, the calculation stops and a DIAGNØSTIC notifies the user about the nature and location of the error. A complete list of DIAGNØSTICS is given in Section 4.4.

Calculation Option (IØPT9)

The calculation c the coordinate system may be stored on a data file and retrieved for use in subsequent cases. If IØPT9=1, both the coordinates and the viscous flowfield are calculated. If IØPT9=2, the coordinate system is calculated and stored on file NINE and the calculation stops. If IØPT9=3, the coordinates stored on file NINE are recalled and the viscous flowfield is calculated. This feature is particularly useful when the user wishes to calculate several flows using the same duct geometry.

Data Files

Since three separate computer codes are used in the analysis, data is passed from one computer code to the other through data files. The ADD code generates the coordinate system and stores the results on file NINE. The ADD code also generates the viscous flowfield solution and stores the results on file EIGHT. Both the PTRACK and VAPDIF codes require the data stored on files EIGHT and NINE. The PTRAK code calculates the rate of evaporation of fuel droplets for use as the source terms for the solution of the diffusion equation by the VAPDIF code. These source terms are stored on file SEVENTEEN. The VAPDIF code uses the data stored on all three files. It is recommended that these files be registered and catalogued files so that the data may be stored permanently over a period of several weeks. Proper use of these files allows the user great flexibility in solving problems.

Start/Stop Options

A flow calculation may be started at coordinate station J=IØPTI5 and it may be terminated at coordinate system station J=IØPTI6. If IØPTI5 is not specified, it is assigned a value IØPTI5=1; if IØPTI6 is not specified, it is assigned a value IØPTI6=JL. The calculation of the flowfield may be continued (or restarted) at the JM coordinate station by specifying IØPTI7=JM.

Turbulence Models (IØPT12)

The ADD code is provided with four turbulence models described in Volume I. For IØPT12= 0, 1, 2 algebraic turbulence models are used based on Prandtl's mixing length theory. For IØPT12=3, a two equation model of turbulence is used. Option IØPT12=0 uses a turbulence model which is well established for equilibrium turbulent flowfields and is therefore recommended for all calculations. The other options (IØPT12= 1, 2, 3) are operation but these models have been applied to only a few flowfield situations; the use of these models is not recommended at the present time.

Blade Force Options (IØPT2) (IØPT5) (IØPT10)

Struts, inlet guide vanes, stators, and rotors are modeled in the ADD code as a-priori body forces. Three options exist in the code for calculating these forces. If measurements of stagnation pressure P_T , swirl angle α , and stagnation temperature T_T are available, the blade forces can be calculated from blade element theory by setting IØPT2=1. If IØPT5=2, the program uses the inlet/exit flow data for IØPT1=4. If IØPT5=1, separate data must be read for the blade force calculation. If IØPT2=3, the blade force is calculated from the flow conditions and blade geometry using blade element theory and empirical cascade correlations. If IØPT2=4, the blade force is calculated using the distributions of exit air swirl angle α_2 (Y) and loss coefficient Z_B (Y).

IØPT10 determines whether the blade is stationary (IØPT10=1, stator) or rotating (IØPT10=2, rotor).

Global Iteration (IOPT14)

The ADD code can treat small regions of separated and reattached flow (a separation bubble) using a global iteration procedure. For these cases, KDS must be specified. The first iteration is made with IØPT14=0. The second and successive iterations are made by repeating the calculation with IØPT14=1. As successive passes (iterations) are made, the solution stored on file EIGHT is updated.

3.2 General Features of PTRAK Code

Program Language

The Particle Tracking (PTRAK) code is written in the FØRTRAN V computer language for use on a UNIVAC 1100/81A computer. Some machine specific language, such as PARAMETER and INCLUDE FØRTRAN statements, is used. However, these statements may be replaced easily by equivalent code for use on other machines. The PTRAK code makes use of a UNIVAC routine NTRAN which stores and retrieves large data blocks on disc files; the PTRAK code is designed so that NTRAN is easily replaced with the equivalent FØRTRAN DEFINE FILE statements by modifying only one subroutine.

Grid Selection

The PTRAK axial and radial coordinates and computational grid are calculated by the ADD code and stored in file NINE. In addition, the PTRAK code uses the viscous flowfield solution generated by the ADD code and stored in file EIGHT. All information required by the PTRAK code, such as number of mesh points (JL x KL), the starting station (JFIRST), and the termination station (JLAST) are also stored on coordinate file NINE. Information on the third (ϕ) coordinate must be input to the PTRAK code. This information consists of the number of azimuthal grid points (LPHI \leq 50), and the azimuthal step size ($\Delta\phi$). Finally the number of axial steps per ADD code streamwise station (KDS) must be specified. The appropriate value of KDS is determined primarily by how capidly both the droplet trajectories and velocities are changing. At the present time, no algorithm to alter the axial step-size automatically exists in the PTRAK code so that KDS must be set to the largest value (smallest step size) required for an accurate solution.

Boundary Conditions (IØPT3)

Two types of boundary conditions are possible: a wall boundary condition or a periodic boundary condition. At a solid wall, a droplet may either strike the wall and remain thereon or it may rebound elastically. Droplets remaining on a wall may undergo additional evaporation. Droplet-solid wall interaction boundary conditions include: elastic rebound with no vaporization (IØPT3=0, 1); elastic rebound with vaporization (IØPT3= 2, 3). A periodic boundary condition is available for swirling flows in annular ducts. Thus if IØPT3= 1 or 3, the duct is assumed to have four rectangular solid walls. If IØPT3= 0 or 2, the duct is assumed to be an annular duct defined by solid walls and two permeable side-walls with periodic boundary conditions such that, if a droplet exits through one side-wall, an identical droplet will enter through the opposite side-wall; therefore, only an annular segment of the flow needs to be analyzed.

Location of Fuel Injectors

Each of several fuel injectors may be placed arbitrarily in the duct at any axial station by specifyiying its coordinates (r, z, ϕ) . The calculation will start at the first computed viscous flowfield station generated by the ADD code. Integration of the droplet equations will not start until the axial station is reached at which the first fuel injector is located; it will continue until all of the fuel droplets have evaporated.

Initial Droplet Condit_ns

The initial droplet conditions for each class of droplets consist of its three initial velocity components, diamete, and temperature; up to 1250 droplet classes may be input. The PTRAK code uses a forward marching calculation procedure so that all droplet classes must have an initial velocity component in the downstream direction. Injection angles are limited, therefore, to values less than 85 deg relative to the axial direction.

Compositon of Fuel Droplets

Droplets of either single component or multicomponent (distillate) fuels may be considered by specifying the appropriate thermodynamic and transport properties described in Section 4.4 of Volume I. For droplets of distillate fuel, it is necessary to provide both a distillation curve and a Cox chart.

Droplet/Droplet Collisions (IØPT1, IØPT2)

Models for droplet shattering (controlled by IØPT1) and droplet-droplet collisions and coalescence (controlled by (IØPT2) are available in the program.

Autoignition Model (IØPT7)

Source terms for the rate of production per unit volume of the critical species for autoignition can be calculated for use subsequently in the VAPDIF code.

3.3 General Features of VAPDIF Code

Program Language

The Vapor Diffusion (VAPDIF) code is written in the FØRTRAN V computer language for use on a UNIVAC 1100/81A computer. Some machine specific language, such as PARAMETER and INCLUDE FØRTRAN statements, is used; however these statements may be replaced easily by the equivalent code for use on other machines. The PTRAK code makes use of a UNIVAC routine NTRAN which stores and retrieves large data blocks on disc files; the PTRAK code is designed so that NTRAN is easily replaced with the equivalent FØRTRAN DEFINE FILE statements by modifying only one subroutine.

Grid Selection

The VAPDIF code uses the coordinates and computational grid generated by the ADD code and stored in file NINE. In addition it uses the viscous flowfield solution generated by the ADD code and stored in file EICHT together with the vapor and critical species source distributions and boundary conditions generated by the PTRAK code and stored in various files. All information required to locate data at corresponding grid points is stored in these files.

Boundary Conditions

The boundary conditions are specified completely by the ADD code and PTRAK code data files.

Initial Conditions

It is assumed that the initial concentration of fuel vapor is zero. However, the user may specify a constant mass fraction CZERO (card 4) which is distributed uniformly over the entire initial plane.

Restart Option

The calculation may be started, terminated, or restarted at any axial station in the duct. These options are controlled by the input parameters IADD, IBEGIN, and IEND on input card 2. The variable IADD is equal to JFIRST from the ADD code calculation. IBEGIN is the first calculation station, not including the initial plane, for the VAPDIF code. Normally, the calculation is started with IBEGIN equal to IADD + 1. IEND is the last calculation station in terms of the ADD code coordinates. If IBEGIN > IADD + 1, the code assumes that the solution has been calculated and stored in file ELEVEN for station IADD up to station IBEGIN-1. Thus by specifying IBEGIN and IEND the calculation can be started and stopped at any point.

Print Options (IPRNTX)

Since the VAPDIF code solves a three-dimensional problem, very large amounts of data are necessary to describe completely the solution. For a maximum of a 100 streamwise stations, 100 normal (radial), and 50 tangential stations, there are 5×10^5 grid points. At each grid point the concentration (C), the three coordinates (n, s, ϕ) , the three metric coefficients, the three physical distances, and the three cartesian coordinates must be specified. Therefore the total number of data points is 6.5×10^6 . Print options (card 3) may be used to limit the data printout. In all cases, however, a summary table is given which includes the fuel vapor flow rate, fuel air ratio, and mass flow weighted average mass fraction of fuel as a function of axial distance.

Autoignition Model

Subsequent to the calculation of the three-dimensional fuel vapor distribution, the Vapor Diffusion code can be used to determine the distribution of critical species and thereby estimate whether autoignition of the fuel vapor-air mixture will occur.

4.0 OPERATION OF THE ADD CODE

4.1 Runstream for ADD Code

It is assumed that:

- 1. The program will be executed in TPF\$;
- 2. The executable (absolute) element is MAPADD;
- A catalogued file exists for storing the viscous flowfield (and is called EIGHT in this example);
- 4. A catalogued file exists for storing the flowfield geometry (and is called NINE in this example).

Then the following runstream is sufficient to execute the ADD code.

@ASG,AX EIGHT.,D/O/TRK/300000 @ASG,AX NINE.,D/O/TRK/250000

@USE 8, EIGHT

@USE 9,NINE

@ASG,T 10,D/O/TRK/6000

@ASG,T 11,D/O/TRK/50000

@ASG,T 14,D/O/TRK/60000

@ASG,T 22,D/O/TRK/300000

@XQT MAPADD

(INPUT CARDS)

@FREE 8

@FREE 9

@FREE 10

@FREE 11

@FREE 14

@FREE 22

Card 8

4.2 Input Format for ADD Code

The input format for the ADD code is described on the input data coding forms which follow. These coding forms are organized with one form per input data card. Each form contains the names of the variables, the format, and a description of the data. The input option card controls the data that must be read. Since not all cards are read, the user should make certain that the input data agrees with the input options.

In general the input data is read as follows:

Card 1	Title Card
Card 2	Option Card
Card 3	Mesh Parameter Card
Card 4	Duct Geometry Card + data as required by IØPT3
Card 5	Inlet Flow Card + data as required by IØPT1
Card 6	Force Data Card (If IØPT2 ≠ 0) + data as required by IØPT2, IØPT5, IØPT10

Slot Flow Data Card (option not available)

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Card 2 OPTION CARD FORMAT (3412)

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The input option parameters IØTP1 through IØPT17 determine program flow options to be executed by the ADD code and determine the input data cards to be read. These options are described on the following These options are The input option parameters IDBG1 through IDBG17 are debug options not normally used. described in Sec. 4.5

IØPT1 (FLØWIN Option)

- = 3 Inlet flow is computed by specifying data on Card 5. (turbulent flow)
- = 4 Inlet and exit flow profiles are read from 2*KLL data cards following Card 5. Input, fractional distance Y, stagnation pressure $P_T(Y)$, static pressure P(Y), swirl angle $\alpha(Y)$, and stagnation temperature $T_T(Y)$. (turbulent flow)
- = 7 Inlet flow is computed by specifying data on Card 5 (laminar flow)
- = 8 Same as 4 but for laminar flow .
- = 9 Same as 4 but: Input fractional distance Y, stagnation pressure $P_T(Y)$, streamwise velocity $U_s(Y)$, swirl velocity $U_{\varphi}(Y)$ and stagnation temperature $T_T(Y)$. (turbulent flow)

I PT2 (FORCE Option)

- = 0 No blade force
- = 1 Calculate blade force from upstream/downstream flow data; input fractional distance Y, stagnation pressure $P_T(Y)$, static pressure P(Y), swirl angle $\alpha(Y)$, and stagnation temperature $T_T(Y)$
- = 2 Not available
- = 3 Calculate blade force from cascade correlations
- = 4 Calculate blade force from fractional distance Y, exit flow swirl angle $\alpha_2(Y)$, and loss coefficient $Z_B(Y)$

IOPT3 (GDUCT Option) Information follows Card 2

- = 1 Calculate a straight, annular duct.
- = 2 Read co-ordinates of duct.
- = 3 Calculate a straight-walled, annular diffuser.

IØPT4 (PRINT Option)

Print solution every IØPT4 station. For example, if IØPT4 = 3, every third station will be printed. If IØPT4 \leq -1, the code provides an extended printout; this extended printout includes information about the boundary layer profiles and the turbulence model.

R82-915362-40

I ØPT5 (STRUT INPUT Option)

Strut input data (if IOPT2 = 1) used to calculate strut forces from experimental data measured upstream and downstream of strut.

- = 1 Read in required profiles.
- = 2 The upstream and downstream strut data cards are identical to the inlet and exit flow cards and are not read.

I ØPT6 (STRUT Thickness Effects)

- 0 Include strut forces plus thickness effects
- Include strut thickness effects only.

IØPT7 Not Used

IØPT8 (PLOT Option)

- = 0 No plots requested.
- = 1 Make CALCOMP plots (not available at LeRC)

IPPT9 (COORDINATE Option)

- = 0 Make an approximate calculation for both streamlines and potential lines--do not save flowfield on disk. Used only for IOPT3=1.
- = 1 Make exact calculation of streamlines and potential lines-store results on logical unit 9 and complete viscous flow calculation.
- = 2 Same as 1 but terminate calculation after coordinate calculations are completed.
- = 3 Read geometry from logical unit 9 and use in viscous flow calculation.

IØPT10 (RØTØR Option)

- = 0 No rotors or stators.
- = 1 Stators are present.
- = 2 Rotors are present.

IØPT11 (FLØW Option)

- = 0 Internal flow.
- = 1 External flow.

IOPT12 (TURBULENCE Option)

- = 0 Use two-layer turbulence model.
- = 1 Use two-layer turbulence model with low Reynolds number correction.
- = 2 Use two-layer turbulence model with streamline curvature correction.
- = 3 Use two equation turbulence model (applicable to flows in annular diffusers only; i.e., diffusers with both inner and outer walls).

IOPT13 (SLOT Option) (Not available)

- = 0 No slot cooling.
- = 1 Slot cooling.

IØPT14 (GLØBAL Option)

- = 0 Global iterations not used.
- = 1 Global iterations used backward differencing for streamwise velocity derivatives in vicinity of separation.

IØPT15 (JFIRST Option)

Start flow calculation at station IOPT15--if omitted, IOPT15 = 1.

IØPT16 (JLAST Option)

Stop calculation at station IOPT16--if omitted, IOPT16 = JL.

IØPT17 (RESTART Option)

Restart a previously generated case at station IOPT17.

NOTE: IOPT9 must be equal to 3 and KDS must be the same value as used in previous run (see Card 3).

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DDS

FØRMAT (E10.5,613)

MESH PARAMETER CARD

Card 3

ADD CODE INPUT

Mesh Distortion Parameter in normal (radial) direction. The parameter will determine now closely grid points are spaced near the wall. If DDS is input as 0.0, the program will determine an appropriate value.	Number of streamlines (3 $\stackrel{<}{-}$ KL $\stackrel{<}{-}$ 100); for most cases, set KL=50.	Number of streamwise stations (3 \le JL \le 100); for most cases set JL=50	Number of steps per station; if KDS=0, the program will determine the smallest KDS value that satisfies the criteria for numerical stability.	Number of input streamlines for inlet flow data (I \emptyset PT1= 4,8,9). Program will interpolate input data on all KL streamlines.	
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data points will be smoothed and interpolated at calculation grid points. Number of duct geometry input points for IOPT3=2. If JLPTS # JL input

Not used.

JLAST

JLPTS

Card 4 DUCT GEOMETRY CARD FØRMAT(8E10.5)
IØPT3=1 STRAIGHT WALL ANNULAR DUCT

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Card 4 DUCT GEOMETRY CARD FØRMAT(8E10.5)
IØPT3=2 READ DUCT COORDINATES

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If not specified KNØTS = 5. The number of knots is used by the least squares spline fitting and interpolation routines Number of nodal points 32 KNøTS 2 33 Length of duct (cm) Z1 KNØTS

when JL # JLPTS

4-10

ADD CODE INPUT

Cards 4a DUCT 0.D. RADIUS CARDS FØRMAT (8F10.5)

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RADII(J) Tip (0.D.) duct radius (cm) at JLPTS equally spaced axial stations (8 entries per card)

Cards 4b DUCT I.D. RADIUS CARDS FØRMAT(8E10.5)
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RD2I(J) Hub (I.D.) duct radius (cm) at JLPTS equally spaced axial stations (8 entries per card)

AUD CODE TRPIT Card

DUCT SECRETAR CAPD FORMAT(BELO.5) 10PT3 =3 STANGHT WALL ANNULAR DIFFUSER

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Length of duct (cm) 21 2H1

Hub radius-station 1 (cm) Tip radius-station 1 (cm) RII

Length of inlet throat (or straight) section (cm)

Hub wall angle (deg.) ZTHRØ ANGH ANGT

Tip wall angle (deg.)

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5 2

FØRMAT (7E10.5, 2F5.0)

INLET FLOW CARD

in

Car

ODE INPUT

ADI

ANH

AMS1 Inlet Mach number ALP1 Inlet swirl angle (deg) DSHI Hub boundary layer displacement thickness (cm) DSTI Tip boundary layer displacement thickness (cm) ANH Hub power law ANT Tip power law ANT Lip power law

Equivalent sand roughness (µm)

NOTE:

If AMS1 is input, WFL will be calculated. If WFL is input, AMS1 will be calculated. For IOPT1 = 4,8,9 code uses data on card 5 (except AMS1 and ALP) and 2x KLL cards If both AMS1 and WFL are input, AMS1 will be calculated. For I@PT1=3,7 code uses data on cards 5 and 7. 2.

following card 5. If WFL is input, the static pressure profile will be adjusted until input and calculated weight flows agree. 78 79 80

INLET/EXIT FLOW DISTRIBUTION FØRMAT(5E10.5) IMPT1 = 4 2*KLL CARDS FOLLOWING CARD 5.

ADD CODE INPUT

Cards 5a

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 r_{H} is hub radius at inlet (exit) station and r_{T} is tip radius at inlet (exit) Normalized distance across duct Y = $(r-r_H)/(r_T-r_H)$, $0 \le Y \le 1$ where station.

Stagnation pressure (atm)

Static pressure (atm) Swirl angle (deg.) PT P AL TT

Stagnation temperature (OK)

Cards 1 through KLL are inlet conditions.

Cards KLL+1 through 2*KLL are exit conditions.

Load cards with increasing Y including Y=0.0 and Y=1.0.

Program uses exit flow data only for plotting. If exit flow data are not available, use inlet flow data.

Cards 5b IN

INLET/EXIT FLOW DISTRIBUTION FØRMAT(5E10.5)
IØPT1 = 9 2*KLL CARDS FOLLOWING CARD 5.

Normalized distance across duct $Y = (r-r_H)/(r_T-r_H)$, 0.0 $^{<}_{Y}$ $^{<}_{\sim}$ 1.0

Streamwise velocity (m/sec) Static pressure (atm)

US P UP

Swirl velocity (m/sec)

TT Stagnation temperature (°K)

NOTE: 1. Cards 1 through KLL are inlet c

Cards 1 through KLL are inlet conditions.
 Cards KLL+1 through 2*KLL are exit conditions

2. Load cards with increasing Y including Y=0.0 and Y=1.0

3. Program uses exit flow data only for plotting. If n available use inlet flow data.

KBLADE

ISHAPE

MUN

Z

ØMEG:

FORCE DATA CARD FORMAT(F10.5,413)

IF IØPT2 > 0

Card 6

ADD CODE INPUT

ORIGINAL PARE NO OF POOR QUALITY

Rotor speed (rpm) **ØMEGZI**

Number of struts in blade row

Airfoil Section LHAPE

NASA 4 digit series airfoil Thin inlet guide vanes

NASA 5 digit series airfoil Arbitrary thickness airfoil

NASA 65A series airfoil = 2 = 4 = 5

NASA 65CA series airfoil

Number of input airfoil sections on stacking line 2 $\stackrel{<}{\scriptstyle \sim}$ NUM $\stackrel{<}{\scriptstyle \sim}$ 20 ME

Number of input data for blade thickness distribution KBLADE

if ISHAPE=4 KBLADE 5 50

ADD CODE INPUT

Cards 6a

R

STRUT DATA CARDS FØRMAT(6F10.5) NUM CARDS FGLLOWING CARD 6 IF IØPT2 > 0

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Radius of input data at blade center line (stacking line) (cm)

Stagger angle (degrees from blade face)

Blade chord length (cm) ALPS CØRD

Blade thickness/chord

THIK PHI ZCL

Blade camber angle (equivalent circular arc camber in degrees)

Axial distance to blade center line (cm)

NUM \$ 20 NOTE:

Load data with increasing RCL 1.

ADD CODE INPUT

Cards 6b BLADE THICKNESS CARDS FØRMAT(8E10.0)
CARDS FOLLOWING CARDS 6a IF ISHAPE=4

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XK(I) Fractional distance along chord line from blade leading

 $0 \le XK(I) \le 1.0 I = 1, KBLADE$

FØRMAT (8E10.5)

CARDS FOLLOWING CARDS 6b IF ISHAPE=4

BLADE THICKNESS CARDS

Cards 6c

ADD CODE INPUT

ORIGINAL PROTES

YK(I) Blade thickness/chord I = 1, KBLADE

ADD CODE INPUT

Card 7 REFERENCE CONDITIONS FØRMAT (2E10.5,5F6.0,3E10.5)

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PRESO	Inlet stagnation pressure	(atm) default (1 atm)	(1 atm)
TEMPO	Inlet stagnation temperature	(^O K) default (288 ^O K)	(288 ^o K)
ACI	Clauser constant	default (0.16)	
AKI	Von Karmen constant	default (0.41)	
API	Van Driest constant	default (26.0)	
PRTI	Prandtl number, turbulent	default (0.70)	
PRLI	Prandtl number, laminar	default (0.90)	
CPRI	Specific heat, constant pressure (cal/gm/°K) default (0.24)	re (cal/gm/ ^C K)	default (0.24
CVRI	Specific heat, constant volume (cal/m/0K) default (0.17)	$(ca1/m/^{0}K)$	default (0.17
VISCRI	Molecular viscosity at 2880K		(g., cm/sec) default (1.7)
NOTE:	1. If not specified, the indicated default value is used.	icated default	ralue is used.
	2. If IMPT1=4,8or9, PRESM and TEMPM may be omitted	d TEMPØ may be c	omitted

4.3 Output Description for ADD Code

The output on each page from the ADD code is largely self-explanatory. A general description of the output by page is given below.

Title Page

This page presents a list of modifications, dates, and report numbers for all changes to the ADD code.

Input Data Page

This page presents all input data including all options and default input values.

Inlet Flow Pages

If IPT1 = 4, 8 or 9, the input data is checked for self-consistency. Both input and derived results are printed on these pages.

Performance Page

Mean and average quantities of the inlet flow which are frequently used to measure or normalize duct performance are printed on this page.

Wall Conditions Page

The coordinates of the hub and tip wall, mass flow bleed, and wall temperature are printed. For adiabatic walls, the wall temperature is not known before the calculation and appears as $T_{\rm W}$ = 0 on the printout.

Wall Geometry Page

This page prints the wall coordinates, wall curvature, and arc length along the walls.

Gap Average Inviscid Flow Pages

The ADD code calculates the inviscid flow field and prints the solution for each streamwise station as determined by the print option IOPT4.

Gap Average Viscous Flow Pages

The ADD code calculates the viscous flow field solution and prints the solution for each streamwise station as determined by the print option IOPT4. The solution appearing on these pages is stored on file EIGHT.

Boundary Layer Coordinate Pages

When IOPT4 < 0, the velocity and shear stress distribution in universal coordinates $U^+(Y^+)$ and $\tau^+(Y^+)$ and the effective turbulent viscosity and thermal conductivity distributions predicted by the turbulence model are printed.

Turbulence Properties Pages

When $I \not\! D PT4 < 0$, the calculated distribution of turbulence kinetic energy, Reynolds stress, Reynolds number of turbulence, and turbulent Richardson number are printed.

Mass Flow Average Page

At the completion of the calculation, a flow summary is given which includes mass flow weighted averages of several variables, pressure recovery coefficient, and pressure loss coefficient.

Wall Surface Conditions Page

This page presents a summary of wall heat transfer conditions including wall friction coefficient, wall temperature, integrated wall area, and integrated heat transfer through the wall.

Wall Radiation Summary Page

This page presents a summary of data required for wall radiation calculations. This output is not applicable for cases in which the ADD code is applied to premixing fuel preparation passages.

Boundary Layer Parameter Pages (Hub and Tip)

These pages summarize the growth of the boundary layer in terms of displacement thickness, momentum thickness, and shape factor.

4.4 Diagnostics for ADD Code

Numerous checks are made during the course of the calculation. If a minor error cours, a DIAGNØSTIC message is printed and the calculation continues. If a fatal error occurs, a DIAGNØSTIC message is printed and the calculation stops. A description of these DIAGNØSTICS is given in this section. The DIAGNØSTIC message is always of the form:

DIAGNOSTIC NO. XX FOR ANNULAR DIFFUSER DECK

where xx refers to one of the errors listed. It should be noted that numerical values printed with the DIAGNØSTIC message will be in dimensionless form or in English units.

IPT3 OUTSIDE RANGE OF ALLOWABLE DUCT OPTIONS

This error is detected in Subroutine ALTMN. The input option must be between $1 \le I \emptyset PT3 \le 6$.

2) No solution exists in AMFOR

This error is detected in Subroutine AMFOR. This subroutine solves the Mach number function

$$N = M(1 + \frac{Y-1}{2})^{\frac{1}{2}} / (1 + YM^2)$$

for M given N. The function has a maximum at M = 1. Hence

$$N(1) = [2(1+Y)]^{-\frac{1}{2}}$$

Solutions do not exit for values of N > N(1).

3) MASS FLOW EXCEEDS THE MAXIMUM MASS FLOW POSSIBLE

This error is detected in Subroutine AMINLT which solves the Mach number function

$$N = M(1 + \frac{Y-1}{2} M^2)^{-\frac{Y+1}{2(Y-1)}}$$

for M given N. This function has a maximum for M = 1 given by

$$N(1) = (\frac{Y+1}{2}) - \frac{Y+1}{2(Y-1)}$$

corresponding to choked flow.

4) ISHAPE AND IMPT2 ARE NOT CONSISTENT

This error is detected in subroutine CASC. For blade and strut calculations use only $I\emptyset PT2=3$ with any ISHAPE, where

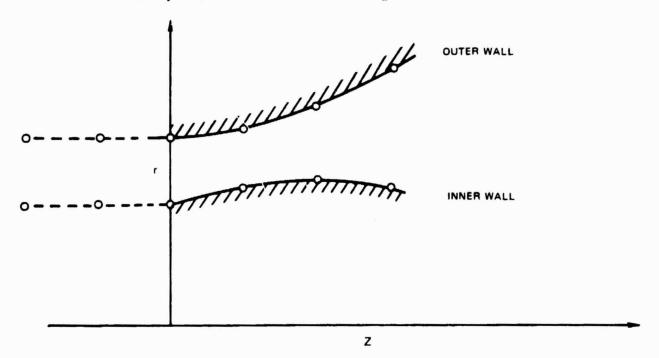
ORIGINAL OF POCR COLLEGE

3 \(\text{ISHAPE} \(\leq \) 6

Otherwise, the calculation will stop.

5) FOR BEST RESULTS ADD A STRAIGHT ANNULAR CHANNEL INLET

This error is detected in Subroutine COOR1. In the construction of the duct coordinates, it is assumed that the inlet has no curvature as shown in the figure below. This is not a fatal error because small inlet curvatures may be tolerated. For best results add a straight annular section to the inlet as shown by the dotted lines in the figure.



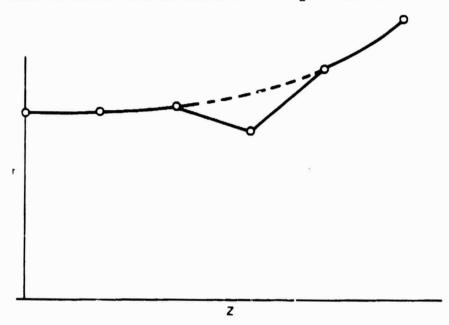
Addition of Straight Annular Channel Inlet

6) PROGRAM ASSUMES INLET FLOW HAS CURVATURE

This error is detected in Subroutine COORL. Same as diagnostic 5.

7) WALL CURVATURE IS TOO LARGE AT STATION X.

This error is detected in Subroutine COORI usually if the duct has a discontinuous change in wall curvature such as shown in the figure below.



Discontinuous Change in Wall Curvature

8) Not Used

9) GREATER THAN 1. PERCENT NORMAL PRESSURE GRADIENT ERROR RECALCULATE STATIC PRESSURE

This error is detected in Subroutine ERPIN. This subroutine integrates the radial momentum equilibrium equation.

$$P_{z} - P_{H} = YM_{r}^{2} \int_{0}^{1} \left| \frac{-p}{V} \frac{\partial V}{\partial n} U_{s}^{2} + \frac{p}{R} \frac{\partial R}{\partial n} U_{\phi}^{2} \right| \frac{\partial n}{\partial v}$$

and compares $(P_T - P_H)$ to that computed for the input inlet flow $(P_T - P_H)_1$. If the error given by

 $E = \left[1 - \frac{P_T + P_H}{(F_T - P_H)_1}\right]$

is greater than 0.01, the input initial static pressure distribution is replaced by the above pressure equation and the inlet flow is recalculated.

10) Not Used

11) MASS FLOW REQUIRED EXCEEDS MAXIMUM MASS FLOW POSSIBLE

This error is detected in Subroutine CKINPT. If it is determined that choked flow exists in the duct, this diagnostic will be printed; the weight flow must be reduced.

12) PRESSURE RISE EXCEEDS PERMISSIBLE PRESSURE RISE

This error is detected in Subroutine CKINPT and indicates that the deck cannot calculate properly the initial flow profiles. Check input for errors.

13) ITERATION OF BACK PRESSURE CALC. FAILS TO CONVERGE

This error is detected in Subroutine FINVIS.

In the calculation of strut forces, it has been assumed that the strut exit flow is subsonic and unseparated (i.e., $U_{\rm g} > 0$). If these conditions are violated, no solution can be obtained. The calculation will stop.

14) BOUNDARY LAYER TOO THIN FOR MESH SPACING

This error is detected in Subroutine FLØWIN. The viscous flow calculation requires a finite initial boundary layer thickness. In addition, it requires enough mesh points to describe the inlet boundary layer velocity profile. The deck assumes arbitrarily that at least five mesh points are required. Thus, if this diagnostic occurs, increase the number of mesh points, KL, increase the mesh distortion parameter, DDS, or increase the assumed inlet boundary layer thickness. If DDS is input equal to zero, the program automatically sets the mesh distortion parameter to the appropriate value for turbulent flow.

15) TOTAL PRESSURE IS LESS THAN STATIC PRESSURE

This error is detected in Subroutine FLOWIN. A check is made on the input data for 10PT1 = 4 to make sure that $P_T > P$.

16) INPUT DATA NOT IN RADIAL EQUILIBRIUM CORRECTIONS APPLIED TO STATIC PRESSURE

This error is detected in Subroutine FLØWIN. A check is made of the input static pressure data for IØPT1 = 4. If the static pressure data are not in radial equilibrium, it is assumed that the static pressure data are in error and that the other inlet data are correct. Then the static pressure profile is computed from

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$$\frac{d\Pi}{d\eta} = 2 \frac{\gamma}{\gamma - 1} \left[\frac{-1}{XV} \frac{\partial V}{\partial n} \cos^2 \alpha - \frac{1}{XR} \frac{\partial R}{\partial n} \sin^2 \alpha \right] \Pi \left(\begin{pmatrix} \Pi_0 \\ \Pi \end{pmatrix}^{\gamma} - 1 \right)^{\gamma}$$

with the ID wall static pressure as a boundary condition.

17) INPUT DDS MUST BE SPECIFIED

This error is detected in Subroutine FNØRM. At this time there is no algorithm to select automatically the mesh distortion parameter DDS for laminar flow.

18) BLADE DATA ERROR IN CKINPT ROUTINE

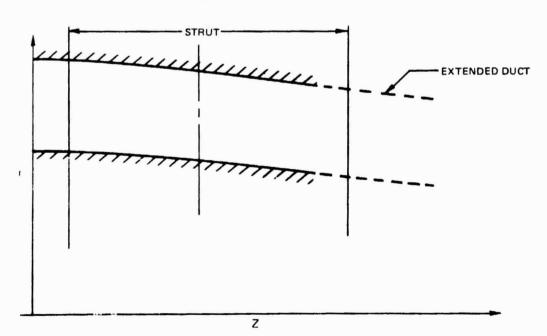
This error is detected in Subroutine CKINPT. Blade data have been input incorrectly and must be rearranged with Y increasing.

19) NO UNIQUE SOLUTION FROM MINVRT

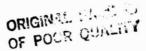
This error is detected in Subroutine MINVRT. If the matrix used to solve for the turbulent flow solution is singular, no solution can be obtained. This situation may occur due to numerical truncation errors.

20) LEADING OR TRAILING EDGE INDEX OF STRUT OUT OF RANGE

This error is detected in Subroutine SLETE. In order to compute blade forces, the strut must be located entirely within the duct length. This problem may be eliminated by extending the duct as shown in the figure.



Extended Duct Section



21) SLOT INPUT NOT IN INCREASING ORDER

This error is detected in Subroutine SLOTA.

The slot input data must be arranged in order of increasing axial distance. Check input data. The calculation stops if this error is detected.

22) CHOKED FLOW IN SLOT NO.

This error is detected in Subroutine SLTFLØ. The slot weight flow is determined by the ratio of the stagnation pressure of the slot coolant fluid to the local wall static pressure. If this pressure ratio is too large the flow may be choked at the slot inlet. The calculation will stop.

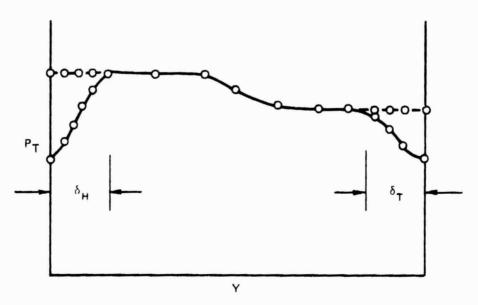
23) BOUNDARY LAYER OVERLAP OR TOO LARGE

This error is detected in Subroutine FLØWIN. For internal flow, the sum of the boundary layer thicknesses on the hub and tip walls must be less than the duct inlet height. Check input data.

24) SET TOTAL TEMPERATURE, PRESSURE, ANGLE TO VALUE AT EDGE OF BOUNDARY LAYER - CORRECTIONS APPLIED

This error is detected in Subroutine FLØWIN. For IØPT1 = 4, the calculated boundary layer profiles are matched to input inlet flow profiles.

A good match requires that the stagnation pressure, $P_{\rm T}$, be constant in the experimentally determined boundary layer region as shown in the figure (dashed line).



Constructing the Inlet Flow

25) TRUNCATION ERROR CANNOT BE REDUCED BY STEP SIZE

This error is detected in Subroutine SØLVI. If the step size parameter (KDS) is not specified, it is selected automatically by checking the truncation error at each step. When an instability occurs, the program attempts to reduce the truncation error by reducing the streamwise step size. If the truncation error cannot be reduced below a minimum value, the calculation stops.

26) NUMERICAL INSTABILITY

This error is detected in Subroutine FCØRCT and Subroutine SØLVI and is an indication that the program has calculated negative temperatures or pressures. The calculation stops if this problem occurs.

27) RHOCX ITERATION DID NOT CONVERGE, ERR =

This error is detected in Subroutine FØRCE. In determining the blade force, an iteration scheme is used to determine the downstream static pressure. If this iteration fails to converge, this diagnostic is printed together with the maximum error found in the iteration. The calculation, however, is not terminated.

28) $I \emptyset PT3 = 2 OPTION NOT IN USE$

This error is detected in Subroutine FØRCE but this option has been deleted from the current version of the ADD code.

29) SOLUTION REQUIRES REVERSE FLOW, INCREASE WFLOW

This error is detected in Subroutine CKINPT. For flows with radial pressure gradients, there is a minimum weight flow below which reverse flow exists. This problem can be corrected by increasing the weight flow. The calculation will stop.

30) LOAD DOWNSTREAM FLOW DATA CARDS

This error is detected in subroutine CALINV and indicates that the downstream flow data cards, required by IOPT1 = 4 or 9, have not been entered. The calculation will stop.

31) SOLUTION FOR BLADE FORCE DOES NOT EXIST

This error is detected in subroutine FØRCE. The blade force cannot be calculated because no inviscid flow solution can be calculated. (Same as DIAGN \emptyset STIC 29) The calculation will stop.

32) GRADIENT OF METRIC COEFFICIENT = FOR BETTER RESULTS ADD STRAIGHT CHANNEL INLET

This error is detected in Subroutine $C \not \! D R 4$. It is assumed that the inlet duct has no curvature. To avoid problems, add a straight annular section to the inlet. The calculation will continue.

33) INPUT TOO LARGE FOR COLE'S LAW SET N < ____

This error is detected in subroutine FLOWIN.

Cole's friction law requires a certain relationship $H_{12} = H_{12}$ (R_e) such that there is an upper bound of n<10. For a solution to exist,

$$A = \kappa \frac{Ue}{U^*} (1 - \frac{1}{H_{12}}) > 1.573$$

Setting

$$H_{\min} = 1 - \frac{\frac{1}{1.5731}}{\frac{\text{KUe}}{\text{U*}}}$$

Then

$$n < \frac{2}{H_{min} - 1}$$

The calculation will stop.

34) WEIGHT FLOW ITERATION MAY NOT CONVERGE IN SUBROUTINE CKINPT CHECK INPUT DATA.

This error is detected in Subroutine CKINPT. The weight flow iteration that determines the static pressure may not converge if the free stream inviscid flow is highly distorted. An input flow which is more uniform in stagnation pressure is required. The calculation will stop.

35) WFLI AND IOPTI1 OPTIONS INCOMPATIBLE

This error is detected in subroutine ALTMN. The weight flow cannot be specified for external flow. The calculation will stop.

36) IOPT1 = 1 OR IOPT1 = 2 OPTIONS NOT USED

This error is detected in Subroutine ALTMN. The options $I\emptyset PT1 = 1$ and $I\emptyset PT1 = 2$ have been deleted from the code.

37) CONFLICT OF OPTIONS, IMPT14<0 IMPLIES SEPARATION AND GLOBAL ITERATIONS. AUTOMATIC STEP SIZE ALGORITHM CANNOT BE USED.

This error is detected in Subroutine SØLVI. When performing a global iteration (IOPT14>0), the same number of streamwise steps must be used for each iteration. Hence the automatic step size algorithm for the streamwise direction must not be used. The calculation will stop.

4.5 Debug Options for ADD Code

When set equal to unity, these options allow intermediate results calculated by the subroutine indicated to be printed as an aid in debugging a troublesome case. Note that these outputs are not converted to metric units and reference must be made to the source code for interpretation of printout.

OPTION	SUBROUTINE	OBJECTIVE OF SUBROUTINE
IDBGI	TURB	Calculates two-layer turbulence model
IDBG2	FCØRCT	Calculates shear stresses and heat fluxes at each station
IDBG3	FLØWIN	Generates initial flow profiles
IDBG4	SLTFLØ	Calculates slot inlet flows
IDBG5	SØLVI	Calculates viscous flow solutions
IDBG6	C Ø ØR	Generates required geometric parameters
IDBG7	FØRCE	Calculates forces generated by struts and blades
IDBG8	MINVRT	Inverts a matrix
IDBG9	SM Ø ØTH	Smooths duct contour read via IPPT3 = 2
IDBG10	GDUCT	Calculates duct geometry
IDBG11	SLTFLØ	Obtains additional information from SLTFL \emptyset - see IDBG4
IDBG12	SØLVI	Obtains additional information from SØLVI - see IDBG5
IDBG13	CKINPT	Checks inlet flow input for errors
IDBG14	SØLVI	Debugs the algorithm that automatically computes the maximum step size in the streamwise direction while assuring computational stability.
IDBG15	Not used.	
IDBG16	Not used.	
IDBG17	Not used.	

4.6 Sample Input for ADD Code

Two sample inputs to the ADD code are presented on the following pages. These cases correspond to the two design studies described in Vol. I Section 7.0. The first sample is the input for the Swirl Tube Premixing Passage Case and the second sample is the input for the Series Staged Premixing Passage Case.

Swirl Tube Premixing Passage

The option card (line 2) indicates that the inlet flow conditions are to be calculated from input flow profile data (IOPT1=9). The duct geometry is to be determined using the straight wall annular diffuser option (IPPT3=3). Only the solution at every 5th station is to be printed (IOPT4=5) and the coordinates are to be read from a previously calculated data file (IØPT9=3). The mesh parameter card (line 3) indicates that the default mesh distortion parameter (DDS = 0.0) and step size (KDS = 0) algorithms are to be used. Two sets of 26 input data cards each describing the inlet and exit flow profiles, respectively, will be read. The duct geometry card (line 4) indicates that the overall duct length is 11.1 cm and that the inlet radius is 2.8956 cm. The inlet flow card (line 5) shows that the initial boundary layer displacement thickness is 0.029 cm and that a 1/7 power law profile is assumed for each wall. Lines 6 through 31 are the KLL=26 inlet flow profile data cards and lines 32 through 57 are the KLL-26 exit flow profile data cards which are identical to the inlet flow cards. The last card indicates that default values are used for the remaining input parameters excert for the Prandtl number, heat capacities, and molecular viscosity.

Series Staged Premixing Passage

The option card (line 2) indicates that the inlet flow is to be calculated assuming a constant stagnation pressure and stagnation temperature in the core flow (I \emptyset PT1=3). The duct geometry is to be read from input data cards (I \emptyset PT3=2). On the mesh parameter card (line 3), the default mesh distortion parameter (DDS=0) has been selected but the streamwise step size parameter has been input KDS=2. From line 3, it is noted that the duct coordinates at JLPTS=50 equally spaced axial stations are to be read and that the least squares spline smoothing routine will be used (JLPTS \neq JL). The length of the duct is 22.72 cm (line 4). Lines 5 through 11 contain 50 data points for the tip radii and lines 12 through 18 contain 50 data points for the hub radii. The inlet Mach number is 0.102 (line 19), the stagnation pressure is 11.06 atm, and the stagnation temperature is 745K.

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5.0 OPERATION OF PTRAK CODE

5.1 Runstreams for PTRAK Code

Autoignition Model Not Used

It is assumed that:

- 1. The program will be executed in TPF\$;
- 2. The executable (absolute) element is PTRACK7;
- The catalogued files, EIGHT and NINE, exist and have been written into by the ADD code (see ADD code input format);
- 4. A catalogued file exists for storing the fuel vaporization terms for use with the VAPDIF code (and is called SEVENTEEN in this example).

Then the following runstream is sufficient to execute the PTRAK code.

@ASG,AX EIGHT.,D/O/TRK/300000

@ASG, AX NINE., D/O/TRK/250000

@USE 8, EIGHT

@USE 9,NINE

@ASG,T 12,D/700000/TRK

@ASG,T 14,D/60000/TRK

@ASG,AX SEVENTEEN.,D/O/TRK/300000

@USE 17,SEVENTEEN

@ASG,T 18

@ASG,T 19

@XQT PTRACK7

(INPUT CARDS)

@FREE 8

OFREE 9

@FREE 12

OFREE 14

@FREE 17

@FREE 18

@FREE 19

Autoignition Model Used

It is assumed that:

- The program will be executed in TPF\$;
- 2. The executable (absolute) element is PTRACK7;
- The catalogued files, EIGHT and NINE, exist and have been written into by the ADD code (see ADD code input format);
- 4. A catalogued file exists for storing the fuel vaporization terms for use with the VAPDIF code (and is called SEVENTEEN in this example).
- 5. A catalogued file exists for storing the critical species source terms for use with the VAPDIF code (and is called TWENTYSEVEN in this example);
- 6. A catalogued file exists for storing the temperature depression source terms for use with the VAPDIF code (and is called TWENTYEIGHT in this example).

Then the following runstream is sufficient to execute the PTRAK code when using the autoignition model.

@ASG,AX EIGHT.,D/O/TRK/300000

@ASG, AX NINE., D/O/TRK/250000

@USE 8, EIGHT

@USE 9,NINE

@ASG,: 12,D/700000/TRK

@ASG,T 14,D/60000/TRK

@ASG,AX SEVENTEEN.,D/O/TRK/300000

QUSE 17, SEVENTEEN

@ASG,T 18

@ASG,T 19

@ASG,AX TWENTYSEVEN.,D/O/TRK/300000

@USE 27, TWENTYSEVEN

@ASG,AX TWENTYEIGHT.,D/O/TRK/300000

@USE 28, TWENTYEIGHT

@XQT PTRACK7

(INPUT CARDS)

@FREE 8

@FREE 9

@FREE 12

@FREE 14

@FREE 17

GFREE 18

@FREE 19

@FREE 27

@FREE 28

5.2 Input Format for PTRAK Code

A CONTRACT

The input to the PTRAK code is described on the input data coding forms which follow. These coding forms are arranged with one form per input data card. Each form contains the names of the input variables, the format, and a description of the data. In general, the input data is read as follows:

Card 1	Title Card
Card 2	Option Card
Card 3	Fuel Class Description Card
Card 4	Injector Description (ILØC) Cards
Card 5	Initial Velocity (ILØC) Cards
Card 6	Fuel Flow Rate Card
Card 7	Fuel Thermodynamic Constants Card
Card 8	Fuel Thermodynamic Functions (6) Cards
Card 9	Air Thermodynamic Constants Card
Card 10	Air Thermodynamic Functions (3) Cards
Card 11	Mesh Description Card
Card 12	Distillation Curve (IDSTL+1) Cards
Card 13	Collision Data Card
Card 14	Cox Chart Data Cards (ICØX1+1) Cards
Card 15	Autoignition Model Constants (3) Cards

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FORMAT (12A6)

TITLE CARD

Card 1

PTRAK CODE IMPUT

PTRAK CODE INPUT

OPTION CARD

Card

FØRMAT (912)

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7 8 9 • r

(Droplet Shattering Model Option) IMPTI

Shattering Model Not Used

Shattering Model Used

(Displet Coalescence Model Option) IØPT2

No Coalescence 0 = Coalescence Considered

(Droplet Wall Rebound Model Option 1ØPT3

Elastic Rebound, Rectangular Passage, No Vaporization from Walls Elastic Rebound, Annular Passage, No Vaporization from Walls

Elastic Rebound, Annular Passage, With Vaporization from Walls

Elastic Rebound, Rectangular Passage, With Vaporization from Walls

Sidewalls Represent the Lateral Extent of a Segment of an Annular Passage; Periodic (This Option is Boundary Condition on Sidewalls, Vaporization from Annular Walls.

Appropriate for Analyzing a Segment of Swirling Flow in Annular Passages.)

(Fuel Droplet Diameter Distribution Option) IØPT4

Binomial Distribution

Rosin-Rammler Distribution

Profit Co.

The state of the

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Irajectory carcuractons	from ADD Run
Station for Periorming 1	If Omitted, Program will Use "JL" From ADD Run
IMPT5 Last Axial S	

IØPT6 (Friction Drag Option)
= 0 Use Droplet Drag Coefficient Correlations

= 1 Set Drag Coefficients to Zero

IØPT7 (VAPDIF Storage Option)

= 0 No Information Is Stored on Unit 17= 1 Store Vapor Source Terms on Unit 17

Store vapor, critical species and temperature depression source terms (on units 17, 27, and 28, respectively) for autoignition Model I (see

Volume I, Section 8.0)

Same as I&PT7 = 2 but for Model II

u

Note: Debug options are described in Section 5.5

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FUEL CLASS DESCRIPTION CARD

FØRMAT (512)

Number of Classes Per Injector Based 'p n Magnitude of Droplet Velocity. (IVS must be ODD) IVS

(IPHI must Number of Classes Per Injector Based Upon Angle of Normal Velocity Component (a). IPHI

Number of Classes Per Injector Based Upon Angle of Tangential Velocity Component (8). be ODD). ITHE

must be ODD).

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(If I@PT4=0, IDIA must be ODD. Number of Classes Per Injector Based Upon Particle (Droplet) Diameter. If IOPT4 = 1, IDIA 5 20.) IDIA

ILØC * IVS * IPHI * ITHE * IDIA < 1250 Note:

Distribution of the last of th

Properties

D. Application

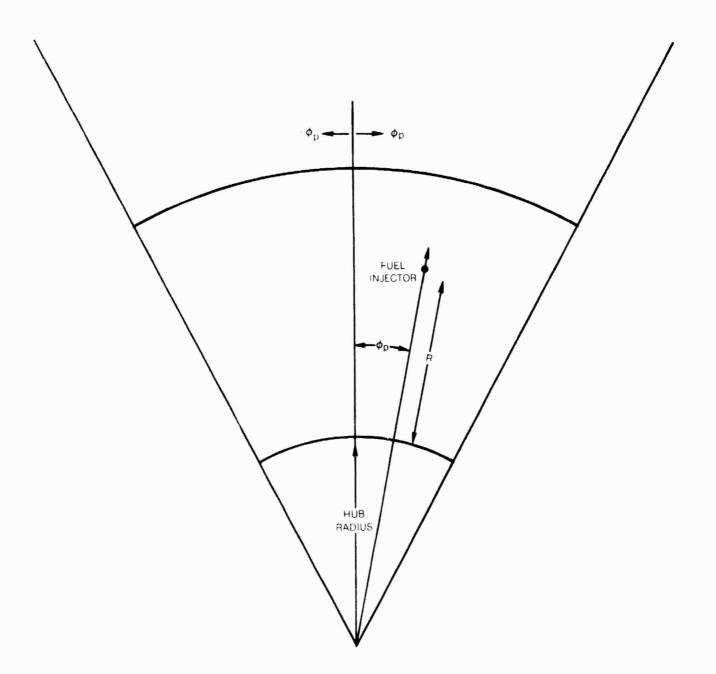
- straction 4.

Law distant

Note: See Fig. 5.1

FUEL INJECTOR DESCRIPTION

(CARD NO. 4)



DDPART

R82-915362-40

Cards

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(microns)

See Fig. 5.2 Note:

Particle Variance (Standard Deviation), Microns - If I@PT4 = 0

DDPART

Mean Particle Diameter if IMPT4 = 0

DPART

DBETA

BETA

Sauter Mean Diameter if IOPT4 = 1

Width Factor (M), Dimensionless - If I pPT4 = 1

DALPHA

ALPHA

DVMEAN

VMEAN

ME AN

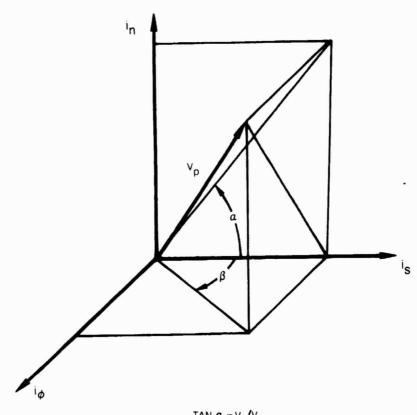
>

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INPUT DROPLET VELOCITY VECTORS



TAN a = Vn/VS TAN $\beta = V_{\phi}/V_{S}$ $V_{MEAN} = |\overrightarrow{V}_{p}|$

R82-915362-40

FØRMAT (8E10.5)

PTRAK CODE INPUT Card 5a

VOLUME FRACTION DISTRIBUTION FOR ROSIN-RAMMLER DISTRIBUTION FUNCTION

Read Enough Cards for IDIA Data Read Only if IOPT4 = 1

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1 2 3

Volume Fraction of Particles of Diameter 2 $_{IK}$ R 1 2 (2) R12(I) R12(

Where At Each Location, The $\stackrel{D}{\text{iK}}_1$ are Calculated From

for I=1, IDIA and K=1, ILOC

and

 Γ (2 - 1/M)

(see Volume I, Ref. 4.21)

Note: $0.0 < R12(I) \le 1.0$

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PTRAK CODE INPUT

Cards 8

FUEL THERMODYNAMIC FUNCTIONS

Read 6 cards

FØRMAT (4E10.5)

Polynomial functions are used to evaluate fuel properties $PROPERTY = A1 + A2*T + A3*T^2 + A4*T^3$ where T = Temperature (deg K)

Units	(gm/cc) (cal/gm/deg K) (gm/cm/sec) (cal/gm/deg K) (cal/cm/deg K/sec) (gm/cm/sec)
Property	Liquid density Liquid heat capacity Liquid heat capacity Natural log of liquid molecular viscosity Vapor heat capacity Vapor thermal conductivity Vapor molecular viscosity
Card	8-1 8-2 8-4 8-5

To dust .

PTRAK CODE INPUT

Cards 10

AIR THERMODYNAMIC CONSTANTS

Read 3 cards

FØRMAT (5E10.5)

0.31.52.51.54.39.56.57.79.39.66.61.67.83.64.80.46		Units	<pre>cal/gm/deg K cal/cm/deg K/sec gm/cm/sec</pre>
7 m 15 70 P 22 23 74 75 75 75 75 75 75 75 75 75 75 75 75 75	ions are used for air properties AT*T + A3*T ² + A4*T ³ T = temperature (deg K)	Property	Air heat capacity Air thermal conductivity Air molecular viscosity
7 • • • • • • • • • • • • • • • • • • •	Polynomial functions are used for air pr PROFERTY = Al + AT*T + A3*T ² + A4*T ³ where T = temperature (deg K)	Card	10-1 10-2 10-3

PTRAK CODE INPUT

Card 11

MESH PARAMETER CARD

FØRMAT (2110, E10.5)

Number of axial steps per ADD code axial station to be used for trajectory calculations KDS

(KDS = 20 is recommended)

Number of grid points used to define the lateral (tangential) extent of the duct (2 \leq LPHI \leq 50) LPHI

"width" of the duct. In this manner, the annular flow field generated by the ADD code Angular step size in tangential direction. The product (LPHI-1)*DPHI is the angular can be subtended by permeable or impermeable sidewalls - See I@PT3 (deg).

See Fig. 5.3

DPHI

Principal P

Descriptions of

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DEFINITION OF LATERAL EXTENT OF DUCT FOR PTRAK

SIDEMAL

(CARD NO 11)

Number o₁ entry points in distillation curve (2 \le IDSTIL \le 20) IDSTIL

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PTRAK CODE INPUT

Card 14

COX CHART DATA CARD

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	43 44 45 46			Pressure for first isobar. PICH must be the same as used to determine the distillation curve (typically, PICH = 1.0 atm).	
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	34 35 36 37 3		(2 ≤ 1	CH must ve (typ	
	30 31 32 33		c Chart	ır. Pl	ar.
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	4 5 6 7	1 C 6 X 1	Н	ρ.,	<u> </u>
١					

PTRAK CODE INPUT

Card 14a

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Carbon number CØX(1)

C (0 X (2)

X

Temperature at vapor pressure PICH for this $C\emptyset X(1)$ CØX(2)

Temperature at vapor pressure P2CH for this $C\emptyset X(1)$ CØX(3)

(deg K)

(deg K)

See Table 5.1 for normal paraffin series Cox Chart In general, $C\emptyset X(3) > C\emptyset X(2)$ at each $C\emptyset X(1)$. $\widehat{\Xi}$ (5) Notes:

Therefo. \circ , the user should enter a sufficient range of $\mathrm{CMX}(2)$ such that the droplet temperature never exceeds the maximum value of CØX(2).

Cox Chart for the Simulation of a Pure Substance

The Cox Chart for simulating a pure substance consists of (a) a set of arbitrary "carbon" numbers, COX(1); (b) a set of arbitrary temperatures for a vapor pressure of P1CH, COX(2); and (c) a set of temperatures all of which are equal to the temperature that produces a vapor pressure of P2CH, COX(3). At any point in the calculation, the program will obtain the distillation temperature for the instantaneous value of percentage of fuel evaporated (this temperature for a pure substance is the normal boiling point), calculate an obviously meaningless "carbon" number, and then find the temperature that produces a vapor pressure equal to P2CH. These parameters are sufficient to calculate the vapor pressure at the instantaneous value of droplet temperature (see Volume I, Section 4.5). A Cox chart for the normal paraffin series is given in Table 5.1.

Characterist of the Control of the C

TABLE 5.1

COX CHART FOR NORMAL PARAFFIN SERIES

P1CH = 1 atm P2CH = 6.8 atm

Carbon No.	T@PlCH (deg K)	T@P2CH (deg K)
2	175	225
3	230	285
4	270	335
5	310	380
6	345	420
7	370	455
8	405	485
9	430	515
10	455	540
11	475	570
12	490	590
13	510	605
14	530	625
15	545	640
16	560	660
17	580	675
18	588	690
19	605	700
20	620	715
23	640	740

Total Control

-

britaning----

PTRAK CODE INPUT

Card 15a

2 3

AUTOIGNITION MODEL CONSTANTS

FORMAT (110,3E10.5)

Number of steps in time-wise integration for critical species source term (typical value, 10) LRUP

For example, if AS is the axial step-size for the ADD code run and Up is the mean particle velocity in AS, then the time-step, δt , for integrating the reaction rate equation for the critical species source term is of the order

AS Up*KDS*LRLP 11 S.

£t should be equal to (approximately) 1 µsec.

Ratio of initial critical species to fuel vapor concentration **DELM2**

(recommended values: 10-4 for Model I, 1.0 for Model II)

Number of carbon atoms in fuel molecule CARBN Mole fraction of oxygen in gas (typical value, 0.21)

Y02

PTRAK CODE INPUT

Card 15b

AUTOIGNITION MODEL CONSTANTS

FORMAT (7E10.5)

Constants for critical species production ("forward") reaction rate expression.

dX2/dt = AF*EXP(-EF/(R*T))*X02**ALPF*XFUEL**BETF*X2**GAMF

*PHI **DELF*T**ANUF

where X02, XFUEL, X2 are concentrations of oxygen, fuel vapor and critical species in mole/cc

Apparent activation energy (cal/mole)

AF Constant such that the units of dX2/dt are mole/cc-sec

EF

1

PTRAK CODE INPUT

Card 15c

•

+ 6 2 -

AUTOIGNITION MODEL CONSTANTS

FORMAT (7E10.5)

DE LB ETB ALPB B ы

Constants for critical species depletion ("backward") reaction rate expression

(see Card 15b)

Note: For Model II, enter a blank card.

5.3 Output Description for PTRAK Code

The output on each page from the PTRAK code is largely self-explanatory. A general description of the output by page is given below.

Title Page

This page presents a list of modifications, dates, and references to all changes to the PTRAK code.

Option Page

This page lists all options used in the PTRAK calculation and the number of classes in each category.

Fuel Injector Page

This page lists the location and initial conditions for all fuel injectors. The total fuel flow rate is also printed.

Fuel Thermodynamic Properties Page

This page presents the thermodynamic data and transport properties for both the fuel liquid and vapor phases.

Air Thermodynamic Properties Page

This page presents both the thermodynamic data and transport properties for the air and the mesh parameters.

Multicomponent Fuel Properties Page

This page lists the data for the distillation curve and Cox chart.

Autoignition Model Constants Page

This page lists all constants used in the autoignition model.

Initial Conditions by Class Page

This page describes the initial conditions, including number density, for all droplet classes.

Duct Geometry Page

This page presents the coordinates of the duct contour.

Solution Pages

These pages present all of the dependent variables by class, and the overall Sauter mean diameter, number of droplets, and fuel flow rate at each axial station.

Summary Page

The summary page presents the global properties of the fuel spray and includes the Sauter mean diameter, liquid fuel flow rate, percentage of fuel evaporated, and fuel-air ratio as a function of axial distance.

5.4 Diagnostics for PTRAK Code

Numerous checks are made during the course of the calculation. If a minor error occurs, a DIAGNØSTIC message is printed and the calculation continues. If a fatal error occurs, a DIAGNØSTIC is printed and the calculation is stopped. A description of these errors is given in this section. The DIAGNØSTIC message is always of the form

DIAGNØSTIC NO. XX FOR PTRAK CODE

where xx refers to one of the errors listed below.

1. FAILURE TO INTERPOLATE IN FINTP

This error occurs when the PTRAK code cannot find the location where a particle track crosses a grid point. The axial step-size should be reduced by increasing KDS. This error causes the calculation to terminate.

5.5 Debug Options for PTRAK Code

When set equal to unity, these options allow intermediate results calculated by the subroutine indicated to be printed as an aid in debugging a troublesome case. These outputs are not converted to metric units and reference must be made to the source code for interpretation of the printout.

OPTION	SUBROUTINE
IDBG1	PTRAK
IDBG2	BØUNCE
IDBG3	CØLLSM, COLLDB

5.6 Sample Input for PTRAK Code

This sample of input to the PTRAK code is based on the Series Staged Premixing Passage case described in Volume I, Section 7. The option card (line 2) indicates that the duct is an annular passage with periodic boundary conditions (IOPT3=4). Thus the inner and outer boundaries are to be treated as solid walls and the two remaining boundaries represent the lateral extent of the annular segment being considered. While the air flow in this case is not swirling, droplets injected normal to the flow direction but in the angular direction may exit from this segment to an adjacent segment. If droplets do exit through one of the "sidewalls", then a source of droplets identical in all respects to this sink of droplets must enter this segment through the opposite sidewall. Only the behavior of the spray in a 1/60th segment of the annular duct is to be calculated (LPHI = 31 and DPHI = 0.2 from line 24). From line 5, the fuel class description card, there are four injectors (ILØC = 4) and only one class is to be formed at each injection location using the binominal distribution function for each property. Thus, the total number of droplet classes is four. These four injectors, described on lines 4 through 7, are located 7.48 cm from the inlet. Lines 8 through 11 describe the initial velocity components and droplet size for each injector. The fuel flow rate is .01146 kg/sec (line 12). The thermodynamic and transport data for the fuel and air are presented on lines 13 through 23. The distillation curve appears on lines 25 through 31 and the Cox chart is listed on lines 33 through 53. All droplets which strike a solid wall will rebound elastically (line 32, Cl = 1.0).

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6.0 OPERATION OF VAPDIF CODE

6.1 Runstreams for VAPDIF Code

Calculation of Fuel Vapor Mass Fraction Distribution

It is assumed that:

- 1. The program will be executed in TPF\$;
- 2. The executable (absolute) element is DIFFUSEMAP;
- The catalogued files, EIGHT and NINE, exist and have been written into by the ADD code;
- The catalogued file, SEVENTEEN, exists and has been written into by the PTRAK code;
- 5. The catalogued file, FUELSEL, exists and will be written into by the VAPDIF code. It is used to permit the VAPDIF code to researt a case subsequent to the initial run. If no restart capability is desired, this file may be a temporary file. The file FUELSØL contains the solution of the diffusion equation at each mesh point for the fuel vapor mass fraction.

Then the following runstream is sufficient to execute the VAPDIF code.

@ASG,AX EIGHT,D/O/TRK/300000

@ASG,AX NIME,D/O/TRK/250000

@USE 8, EIGHT

@USE 9,NINE

@ASG,T 10,D/O/TRK/2250000

@ASG,AX FUELSØL,D/O/TRK/250000

@USE 11, FUELSØL

@ASG,T 12/D/O/TRK/750000

CASG, T 13, D/O/TRK/2250000

@ASG, AX SEVENTEEN., D/O/TRK/300000

@USE 17, SEVENTEEN

@XQT DIFFUSEMAP

(INPUT CARDS)

@FREE 8

@FREE 9

@FREE 10

@FREE 11

@FREE 12

@FREE 13

@FREE 17

Calculation of Critical Species Concentration Distribution

The mass fraction of critical species (ethene when using autoignition Model I) or of the <u>relative</u> mass fraction of the unknown critical species (using autoignition Model II) can be calculated using the following runstream once the fuel vapor mass fraction distribution is known.

It is assumed that:

- 1. The program will be executed in TPF\$;
- The executable (absolute) element is DIFFUSEMAP;
- The catalogued files, EIGHT and NINE, exist and have been written into by the ADD code;
- 4. The catalogued files, SEVENTEEN, TWENTYSEVEN and TWENTYEIGHT have been written into by the PTRAK code;
- 5. The catalogued file, ELEVEN, exists and will be written into by the VAPDIF code. It is used to permit the VAPDIF code to restart a case subsequent to the initial run. If no restart capability is desired, this file may be a temporary file. The file ELEVEN contains the solution to the diffusion equation at each mesh point for the concentration of critical species.
- 6. The catalogued file, FUELSØL, exists and contains the fuel vapor mass fraction distribution determined previously by the VAPDIF code.

Then the following runstream is sufficient to execute the VAPDIF code when using the autoignition model.

@ASG,AX EIGHT,D/O/TRK/300000

@ASG,AX NINE,D/O/TRK/250000

@USE 8, EIGHT

@USE 9, NINE

@ASG,T 10,D/O/TRK/2250000

@ASG,AX ELEVEN,D/O/TRK/250000

@USE 11, ELEVEN

@ASG,T 12/D/O/TRK/750000

@ASG,T 13,D/O/TRK/2250000

@ASG,AX SEVENTEEN.,D/O/TRK/300000

@USE 17.SEVENTEEN

@ASG, AX FUELSØL., D/O/TRK/250000

@USE 19, FUELSØL

@ASG,AX TWENTYSEVEN.,D/O/TRK/300000

@USE 27, TWENTYSEVEN

@ASG, AX TWENTYEIGHT., D/O/TRK/300000

@USE 28, TWE! TYEIGHT

@XQT . DIFFUSEMAP

(INPUT CARDS)

@FREE 8

@FREE 9

@FREE 10

@FREE 11

@FREE 12

@FREE 13

@FREE 17

@FREE 19

@FREE 27

@FREE 28

Attain bentaming

6.2 Input Format for VAPDIF Code

The input to the VAPDIF code is described on the input data coding forms which follow. These coding forms are arranged with one form per input data card. In general the input data is read as follows:

Card 1	Title Card
Card 2	Option Cara
Card 3	Print Option Card
Card 4	Miscellaneous Data Card
Card 5	Autoignition Model Constants (4) Cards

6-6

VAPPIF CODE INPUT

Card 2

OPTION CARD

FØRMAT (4012)

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Maximum number of iterations per station (5 if omitted, 20 is recommended) IØPT1

Starting station in terms of ADD coordinate axial station numbering system; initial plane (or station) for vapor diffusion (VAPDIF) code. Normally, IADD

IADD = JFIRST

First calculation station for the VAPDIF code in terms of ADD coordinate axial IBECIN

station numbering system.

Normally, IBEGIN = IADD + 1 3

If this is a restart of a previously case (see IEND, below), (5)

IBEGIN > IADD + 1

Last calculation station for the VAPDIF code in terms of ADD coordinate axial station numbering system. IEND > IBEGIN and may be used to stop program to examine output. IEND

Normally, IEND = JLAST Then program may be restarted using IBEGIN. Maximum number of coordinate axial stations. If omitted, IL is set equal to value of JL from ADD file (Unit 9). IL

O Do not adjust calculated mass fraction to give agreement with PTRAK integrated 1ØPT8

1 (Recommended) Adjust calculated mass fraction profile - especially useful when source terms are relatively large.

Debug options are described in Section 6.5. NOTE:

FØRMAT (611)

PRINT OPTION CARD

•

Card 3

VAPDIF CCDE INPUT

ORIGINAL PAGE IS OF POOR QUALITY

= 3 Print cartesian coordinates

- See IPRNT2 = 1 Print coordinates (Y, H, y)

No print of the following:

0 #

3

= 1 Print Y (calculation coordinates) = 2 Print H (metric coefficients) Print y (physical distances)

No print of the following:

0

1 Do noc print mass fractions

= 0 Print mass fractions

[PRNT]

IPRNT2 and IFRNT3 produce large volumes of printout - use sparingly

IPRNT4

= 0 No print
= 1 Print interior vapor source terms (from PTRAK)

= (No print 1PRNT5 1 Print boundary vapor source terms (from PTRAK)

= 0 No print 1PRNT6 = 1 Print ADD code flow field

VAPDIF CODE INPUT

Card 4

MISCELLANEOUS DATA CARD

FØRMAT (5E10.5)

RO CZE S E P SCH M DT

Turbulent Schmidt number. SCHMDT

EPSC

Maximum residual for convergence. Let C^V and c^{V+1} be the local concentrations for

iterations v and v+1. The solution has converged when

MAX ($|c^{v+1}-c^v|$) < EPSC * c^v

Let the residual be MAX $(\left|\frac{c^{v+1}-c^{v}}{c^{v}}\right|)$. If omitted, EPSC = 1.0×10^{-5}

Then for successive iterations, the solution is considered to have converged if |RV+1 - RV | < AM. That is, even if the residual is not less than EPSC, the solution has converged if the change in the residual is less than AM.

If omitted, $\Delta M = 1.0 \times 10^{-3}$

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M

Part of the last o

3.

Relaxation parameter. If omitted, the value is obtained from an equation due to Garabedian:

$$Wr = \frac{2}{1 + \lambda \tilde{h}/A^{1/2}}$$

where

$$\hat{h} = \left(\left(\frac{v_{2L}}{J_{L-1}} \right)^2 + \left(\frac{v_{3L}}{\kappa_{L-1}} \right)^2 \right)^{1/2} \\
A^{1/2} = \left(v_{2L} * v_{3L} \right)^{1/2}$$

$$\lambda = 2.53878$$

A value of WR = 1.0 is recommended.

CZERØ

Initial, uniform level of fuel vapor mass fraction in entrance plane.

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VAPDIF CODE INPUT

Card 5a

AUTOIGNITION MODEL CONSTANTS

FORMAT (213)

SCHAK

= 0 Fuel vapor diffusion calculation only ISDC

= 1 Use Autoignition Model I (see Volume I, Section 8.0)

2 Use Autoignition Model II

ISGMAX

model (10 if omitted). If As is the axial step and U is the mean flow velocity Number of time steps in integration of reaction rate equation for autoignition within this step, then the residence time per step is $\Delta t = \Delta s/u$ so that the integration step-size, &t, for the reaction rate equation is

 $\delta t = \Delta t / ISGMAX.$

If ISDG = 1, set ISGMAX large enough such that &t * 1 usec

If ISDG = 2, set ISGMAX = 1 since dX2/dt is not a function of X2.

6-12

VAPDIF CODE INPUT

Card 5c

7

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AUTOIGNITION MODEL CONSTANTS

FORMAT (7E10.5)

1 범 AME B ETF PF 1 Ŀ E-J A

Constants for critical species production ("forward") reaction rate expression

dx2/dt = AF*EXP(-EF/(R*T))*X02**ALPF*XFUEL**BETF*X2**GAMF

*PHI**DELF*T**ANUF

X02, XFUEL, X2 are concentrations of oxygen, fuel vapor and critical species in mole/cc where

Apparent activation energy (cal/mole)

FF

AF

Constant such that the units of dX2/dt are mole/cc-sec

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VAPDIF CODE INPUT

Card 5d

12345678910112131415161718

AUTOIGNITION MODEL CONSTANTS

FORMAT (7E10.5)

rate expression
rate
reaction
n ("backward") reaction rate ex
1 species depletion ("b
species
nstants for critical
for
Constants

(see Card 15b)

Note: For Model II, enter a blank card.

6.3 Output Description for VAPDIF Code

The output on each page from the VAPDIF code is largely self-explanatory. A general description of the output by page is given below.

Input Page

The input page presents all of the input data including: options, computational grid size controls, iteration parameters, and the axial coordinates of the corner point (J = 1, K = 1). In addition the reference conditions for the ADD code viscous flow field are printed.

Source Term Pages

If IPRNT4=1, the source terms on the crossplane grid are printed. These terms are arranged by (K row), (J column) where K is the index for the tangential (azimuthal) coordinate and J is the index for the normal (radial) coordinate.

Solution Page

If IPRNT1 = 0, the mass fractions on the crossplane grid are printed.

Coordinate Grid Page

For IPRNT2 or IPRNT3 # 0, the coordinates on the crossplane grid are printed.

Iteration Page

If IDB1 = 1, the iteration history of the calculation is printed. This printout includes the iteration number, residual, maximum concentration, and mass flow weighted average concentration for each residual.

Flow Summary Page

This page presents values of vapor flow rate and vapor fuel to air ratio as a function of axial location determined by integrating the vapor concentration over the crossplane grid at each axial station. The last column, labeled CTIL, is the overall vapor fuel to air ratio as determined by the PTRAK code and serves as a check of the accuracy of the VAPDIF calculation.

6.4 Diagnostics for VAPDIF

- Adjust - 4

At the present time no diagnostics exist for the VAPDIF code.

6.5 Debug Options for VAPDIF Code

If the options IDB1, IDB2, IDB3 are set equal to unity, intermediate results are printed for each iteration.

Optio :	Data Printed
IDB1	Print maximum iteration residuals
IDB2	Not used
TDR3	Print coefficients of linearized equations

The solution for each iteration at the point (J1DBG, K1DBG) on the calculation plane (crossplane grid) may also be printed. These terms are arranged by (K row), (J column) where K is the index for the tangential (azimuthal) coordinate and J is the index for the normal (radial) coordinate. Solutions for the points (J2DBG, K2DBG), (J3DBG, K3DBG), and (J4DBG, K4DBG) may also be displayed.

It is recommended that IDB1 be set equal to unity.

6.6 Sample Input for VAPDIF Code

The sample of input to the VAPDIF code is based on the Swirl Tube Premixing Passage case described in Volume I, Section 7. Since almost all input data required to run the code is stored in data files generated by the ADD and PTRAK codes, little input is required by the VAPDIF code. On card 2 (line 2), it is noted that the number of iterations is limited to IPPT1=5. The initial flowfield station is located at the first ADD code coordinate station (IADD=1), the first calculation station after the initial plane is IBEGIN=2, and the calculation will terminate at station IEND = 5. The print option card (line 3) indicates that both the concentrations and fuel source distributions will be printed at each station. The last card (line 4) shows that the Schmidt number is unity.

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VAPOR DIFFUSION CASE FOR PARAMETRIC CASE 1000100

-CM4

7.0 GLOBAL STRUCTURE

7.1 Interaction of ADD, PTRAK, VAPDIF Codes

The Global Structure Flow Chart which describes the interactions of the ADD, PTRAK, and VAPDIF codes is shown on Fig. 7.1. The three codes are executed independently in the sequential order shown and output stored on data files. The data files (Units 8, 9, 11, 17, 19, 27, 28) are the only interfaces between the codes.

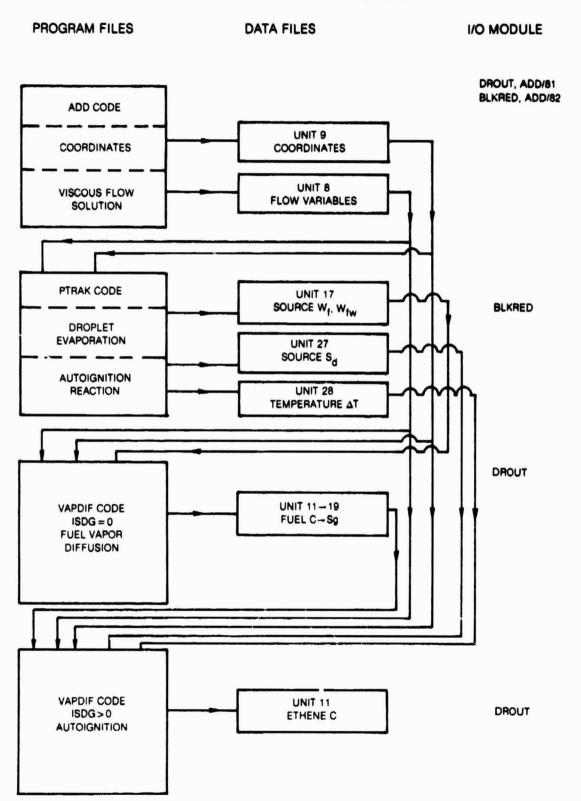
The ADD code calculates the computational coordinates (S,N) and physical cylindrical coordinates (r,z) and stores this data on Unit 9. This coordinate data is required by both the PTRAK and VAPDIF codes. The ADD code also calculates the viscous flow solution and stores the flow variables (P,T, ρ , \vec{V} , μ_E) on Unit 8. These flow variables are required by both the PTRAK and VAPDIF. Certain control parameters, such as the number of streamlines KL and number of streamwise stations JL, which are required by the PTRAK and VAPDIF codes are also stored on Units 8 and 9 and are not required inputs to these codes. This procedure reduces conflicts or ambiguities when executing the three codes.

The PTRAK code calculates the droplet trajectories and degree of evaporation from the initial droplet conditions and known flow field. This solution is used to calculate the source terms W_f and W_{fw} which are stored on Unit 17 for use by the VAPDIF code. The PTRAK code also calculates preignition reactions and stores a source term S_d on Unit 27. As the droplets evaporate, they cool the surrounding air. This temperature drop ΔT is stored on Unit 28.

The VAPDIF code can be executed in two modes. The first execution, with ISDG=0, calculates the three dimensional fuel concentration throughout the flow field using the fuel source distribution calculated from the PTRAK code. This solution is written on Unit 11. On the second execution, ISDG=1 or 2, VAPDIF calculates the concentration of critical species. The fuel concentration which was previously written on Unit 11 is read on Unit 19 and used to calculate the source term due to chemical reaction in the gas phase. The critical species concentration is then stored on Unit 11.

It is noted that all control parameters are calculated and stored by the first code and are not required input to succeeding codes. This arrangement of codes produces considerable flexability in that any data which is calculated and permanently stored on data files need not be repeated. As an example: for any given premixing duct and airflow conditions, several different droplet ejectors may be examined using the PTRAK code without repeating the ADD code calculation.

GLOBAL STRUCTURE FLOW CHART



7.2 Input/Output Data Files

The output data files for the ADD; PTRAK, and VAPDIF codes are described on Tables 7.1, 7.2, 7.3 respectively. These tables show the Unit number, the names of the arrays stored on the file, the block (record) length in words, the number of blocks (records), and the subroutine generating the files. All unit numbers are set by parameters statements (in brackets). All arrays are single precision except AFF generated by the ADD code.

In the operation of the ADD code, only files assigned to Units 8, 9, 11, and 22 are required. The other files are only used for special options in the ADD code which would not generally be used for a LPP duct calculation. Note also that only output files are shown under the computer code name. Input files for the PTRAK code are described on Table 7.1, and input files for the VAPDIF are described on Tables 7.1 and 7.2. The actual file assignments and cunstreams for each code are described in Sections 4.1, 5.1, and 6.1.

These data files are read/written by general I/O routines DRØUT in the ADD/81 and VAPDIF codes or by BLKRED in the ADD/82 (Ref. 4) and PTRAK. These subroutines use the UNIVAC Library I/O routine NTRAN. Both DRØUT and BLKRED are easily converted to ANSI standard FØRTRAN DEFINE FILE.

Table 7.1

Table of File Assignments ADD Code

UNIT NO.	ARRAY NAME	BLOCK LENGTH (WDS)	NO. BLOCKS	SUBROUTINE WRITING BLOCK
8 (NDRUM)	F(NEQ,3,IST) FPARM(15)	3015	JL-2	SØLVI
9(JDRUM)	JSTEP Q(19, IST) RHS(10) RMS(10) RTS(10) DSTEP QPARM(9)	1941	JL	CØØRST
10(CDRUM)	FF(17,2,IST)	3400	1	Parce
11 (LDRUM)	AFF(LNGTO) **	6000	5	SØLVI
12(LFØRC)	FØRC	780	1	FØRCE
19(KPØIS)	JSTEP Q(19,IST) RHS(10) RMS(10) RTS(10) DSTEP QPARM(9)	1941	JL	CØØRS1'
22 (MDRUM)	FIV(NEQ, 3, IST) FIPARM(15)	3015	JL-2	CALINV
23(NFDRM)	F(IST4)	104	JL+NST-2	PØISCF
24 (NPDRM)	P(IST)	100	JL+NST-2	PØIS
25 (NGDRM)	BLK (NGIST)	400	JL+NST-2	PØISCF

^{**}Double precision variables

¹S = 1.00

NST = 25

IST = 100

Table 7.2

Table of File Assignments PTRAK Code

UNIT NO.	ARRAY NAME	BLOCK LENGTH (WDS)	NO. BLOCKS	SUBROUTINE WRITING BLOCK
12(KTDRUM)	PART(200,13)	2600	JL	SMTER
17(MDRUM)	AMASS(IST,50) RDUM(IST,4) APARM(10)	5410	JL	DATAM
18(NBØUN)	RPART(IST,2) PHPART(IST,2)	400	JL	SMTER
19(ISDRU)	SARRAY(8)	8	JL	SMTER
27(MDRUK1)	AMASS(IST,50) RDUM(IST,4) APARM(10)	5410	JL	DATAM
28(MDRUM2)	AMASS(IST,50) RDUM(IST,4) APARM(10)	5410	JL	DATAM

JL = 18 - 100

KL 5 IST = 100

Table 7.3

Table of File Assignments VAPDIF

UNIT NO.	ARRAY NAME	BLOCK LENGTH (WDS)	NO. BLOCKS	SUBROUTINE WRITING BLOCK
10(IYDRM)	Y(3,3,IST,10)	45,000	JL	ADDCØR
11(IFDEM)	FG(IST,10)	5,000	JL	SØLVE
12(IXDRM)	X(3,IST,10)	15,000	JL	ADDC Ø R
13(ITCØR)	TCØR(3,3,1ST,10)	45,000	JL	ADDC Ø R

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8.0 DETAIL DESCRIPTION OF PTRAK CODE

8.1 Main Program/Flow Chart

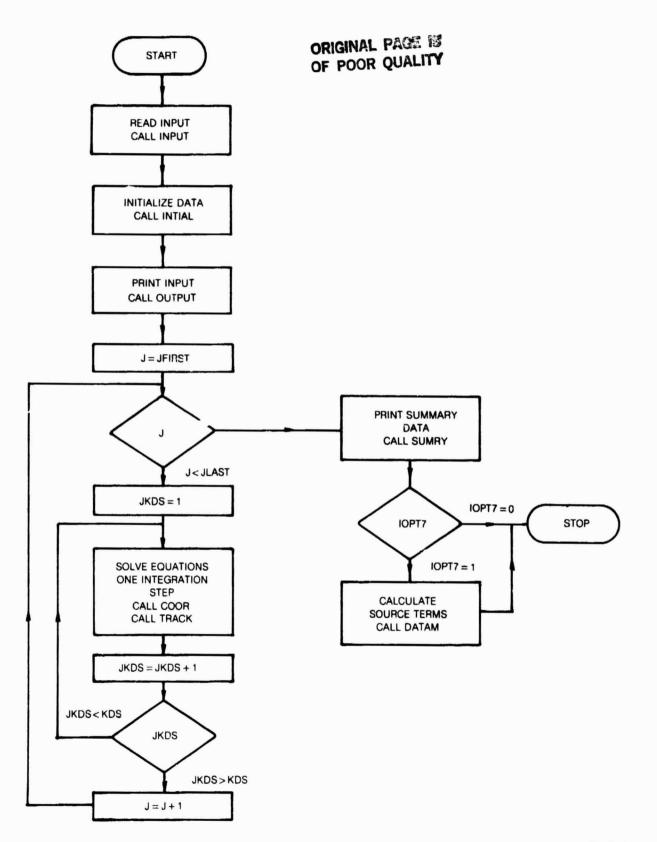
The flow chart for the main program PTRAK is shown on Fig. 8.1. It consists of three major tasks: 1) Read input data and set up initial conditions for the droplet (subroutines INPUT, INTIAL, ØUTPUT); 2) Calculate the droplet trajectory, evaporation rate, and production of critical species (subroutines TRACK, SUMRY); and 3) Calculate the source terms for use by the VAPDIF (subroutine DATAM).

In task 1, INPUT reads the input data according to the input format described in Section 4.2. INIT determines the initial droplet conditions (location, temperature, velocity, mass) which define the droplet classes by specifying number density distribution described in Section 4.7. ØUTPUT prints the input data and initial conditions.

The integration of the droplet equations for one step is accomplished by subroutine TRACK using a fine coordinate grid interpolated from the course coordinate grid calculated by COOR. The outer DO loop indexes the course grid where the J index corresponds to the Jth streamwise coordinate (block) stored on file 9. The inner DO loop indexes the fine grid in KDS interpolated steps using the index JKDS. The integration takes place from JFIRST to JLAST in KDS*(JLAST-JFIRST) steps. At the present time there is no algorithm for varying the step size KDS. As the integration proceeds, the solution at each Jth station for the droplet dependent variables is stored on file 12 and a summary of this data is stored on file 19. When the integration is complete, a summary of the solution is printed by SUMRY.

The execution of the third major task depends on the input option IØPT7. When IØPT7>0, subroutine DATAM searches through the solution files (8,9,12) calculates the source terms for the production of fuel, the source terms for the production of critical species, and the drop in air temperature due to droplet evaporation. These results are stored for each mesh point on the course grid corresponding to the coordinate grid stored on file 9.

FLOW CHART FOR MAIN PROGRAM PTRAK



8.2 Description of Modules by Major Task

A complete list and brief description of all the subroutines is given in Section 8.3. The flow chart for the main program PTRAK is shown on Fig. 8.1 and an overall description is given in Section 8.1. The description of the module functions will follow this flow chart. Only major computational tasks will be described. Minor tasks and Input/Output are self explanatory and will not be described.

Following through the flow chart Fig. 8.1, the first major task is performed by subroutine INTIAL which stores the crossection boundary at the initial station on unit NBØUND, reads the flow field variables at the initial station from unit NDRUM, and calculates the initial droplet conditions by calling subroutine FNØZ. FNØZ specifies the initial conditions (Eqs. 4.7.1), and specifies the number density in phase space defined by (Eq. 4.7.2). Generally the binomial distribution (Eq. 4.7.3) calculated by FBIN is used. At the user's option, the Rosin-Rammler distribution (Eq. 4.7.10) may be used to determine the distribution of droplet diameters.

The second major task is integrating the droplet equations and calculating the droplet collision interactions. Subroutine TRACK performs this calculation for one time step. The flow chart for TRACK is given on Fig. 8.2 which shows the breakdown of the major task into eight smaller tasks. At the beginning of each station on the course grid (J station) IPR=1, the droplet data is read from unit KTDRUM and the flow field variables from unit NDRUM. For each step on the fine grid (JKDS>1) and IPR=0, and the flow field and coordinate variables are interpolated.

The droplet class is defined by the index IJK calculated from the nested DØ loop indices. Thus for each droplet, the droplet motion is calculated by PARPAT, a determination is made if the droplet hits a boundary by WALLRB, and depending on the options IØPT1 and IBREK, a determination is made on whether the droplet shatters by BREKUP, and whether the droplet is a member of the two largest classes by LØCGRD. When the solution for all the droplets at the new time step is determined, LØGCØL examines the two largest classes and applies the collision model. The solution is then printed by subroutine PRINT and stored by subroutine SMTER.

The equations of droplet motion are contained in PARPAT which are integrated for one time step using the predictor corrector method described in Section 4.11. Table 8.1 shows a breakdown of the tasks performed by PARPAT. FINTP locates the droplet on the computational grid and interpolates the flow field variables at that point. FPRØP, GPRØP, and PPRØP calculates the thermodynamic and transport properties for the film, air, and, liquid respectively. DIFFUS calculates the mass diffusion coefficient (Eq. 4.4.16), PØLY is a polynomial interpolation, CØXCH is the Cox chart (see Section 4.5). DRAGF contains the drag coefficient correlation (Eq. 4.2.8) and NUSSET contains the Nusselt number correlations (Eqs. 4.4.1, 4.4.2) for heat and mass transfer. VAHR calculates the heat and mass transfer rates (Eqs. 4.3.4 and 4.3.1). The equations of motion (Eqs. 4.2.1 through 4.2.6) are programmed directly

using DRAGF. The role of change of droplet temperature (Eq. 4.3.3) and droplet diameter (Eq. 4.3.9) is calculated by DTEMP and DDIAM respectively. When the predictor corrector iteration converges (Eq. 4.11.10) the time step is known and the calculation of critical species is made. X2INIT calculates the initial distribution of critical species in the film surrounding the droplet. X2INIT requires VAHR and PFILM to calculate the local partial pressure. XX2 integrates the rate equation (Eq. 8.3.1) using XRATE. X2MASS integrates over the film volume to obtain the mass of critical species (see Eq. 8.2.6). Finally the total heat input to the droplet (see Eq. 8.2.11) is calculated.

The third task in TRACK (Fig. 8.2) is to examine the droplet to see if it hits a boundary using subroutine WALLRB. For purely elastic wall rebound, the velocity component normal to the wall is changed in sign. For periodic boundary conditions, a droplet leaving one boundary enters on the opposite boundary. A portion of the droplets may stay on the wall and form a liquid film. These conditions are calculated by subroutine BØUNCE. BØUNCE determines the fraction of droplets that remain on the wall using the models described in Section 4.10. Of the fraction that remains on the walls, some portion will evaporate depending on the wall temperature and partial pressure calculated from the Cox chart using subroutine CØXCHT as described in Section 4.10.

The next step is to determine if a droplet shatters using subroutine BREKUP and the models discribed in Section 4.9. The droplet shattering model is applied to all classes. After shattering the droplets are counted with the nearest class rather than forming new classes. However, the two largest classes in each computational grid must be recalculated using LØCGRD.

Once the new droplets conditions are established for all classes (IJK loop completed), the droplet collision model LØGCØL can be applied. LØGCØL searches through the computational grid and determines if the two largest classes are in the same grid volume. If they are in the same grid volume, subroutine CØLLDE determines if a collision occurs, and the conditions after a collision using the model described in Section 4.8. A fraction of the droplets may coalesce and a fraction may rebound with elastic collisions. Of those that rebound, subroutine CØLLSN calculates the approach velocity along the line of centers and subroutine CØLDYN calculates the rebound velocity. Subroutine CØLLSN contains the velocity transformation matrix and its inverse to go from the computational coordinates to the collision coordinates. Following the collision, the new properties of the classes are calculated in CØLLDE. The solution is printed by PRINT and stored on files NBQUND, ISDRV, KTDRUM, by SMTER at each Jth station of the course computational grid. This last step completes the calculation in TRACK.

Returning to PTRAK, Fig. 8.1, the calculation continues until the outer $D\emptyset$ loop is completed. An output summary is printed for all J stations on the course grid by subroutine SUMRY. Depending on the input option $I\emptyset PT7$, the source terms are calculated by DATAM. DATAM searches through all the solution files and calculates

the source terms W_f and $W_{f,w}$ for the vapor diffusion equation (Eq. 5.2.1) using Eqs. 4.7.14 and 4.7.15. This result is stored on file MDRUM. It then calculates the source term S_d for the critical species equation (Eq. 8.2.1) using Eq. (8.2.6) and stores the result on file MDRUM1. Finally it calculates the temperature drop due to evaporization and stores the results on file MDRUM2. At this point the calculation in PTRAK is complete.

FLOW CHART FOR SUBROUTINE TRACK

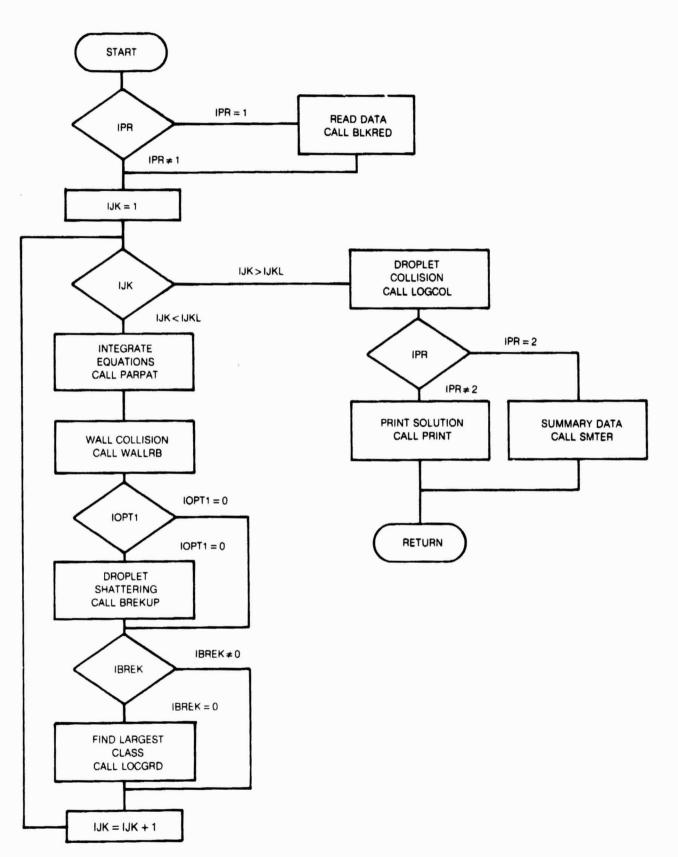


Table 8.1

Tasks in Subroutine PARPAT

Subroutine	Task	Aux. Subroutines
FINTP	locate droplet on grid	
	find local air flow conditions	
FPRØP	film properties (Eqs. 4.4.6 to 4.4.20)	DIFFUS
GPRØP	air properties	PØLY
PPRØP	liquid properties (Eqs. 4.4.21 to 4.4.28)	POLY, CØXCH
DRAGF	drag coeff. (Eq. 4.2.8)	
NUSSET	Nusselt No. (Eq. 4.4.1, 4.4.2)	
VAHR	determine heat transfer (Eq. 4.3.4)	
	determine mass transfer (Eq. 4.3.1)	
	Equations of motion (Eqs. 4.2.1 to 4.2.6)	
DTEMP	Rate of temperature change (Eq. 4.3.3)	
DDIAM	Rate of diameter change (Eq. 4.3.9)	
X2INIT	Initialize critical species	VAHR, PFILM
XX2	Integrate rate equation (Eq. 8.3.1)	PFILM, XRATE
X2MASS	Integrate mass (bracket Eq. 8.2.6)	
	Integrate bracket (Eq. 8.2.11)	

8.3 List of Subroutines in PTRAK

ALJPØT Evaluate Leonard Jones Potential collision integral

BLKDAT Block data

BLKRED Read/Write data on files

BØUNCE Wall rebound model

BREKUP Droplet Shattering model

CØLDYN Calculate droplet velocity after collision

COLLDE Droplet Collision model

CØLLSN Calculate velocity transformation matrix

COOR Read coordinate data

CØXCHT Determine vapor pressure from Cox chart

DATAM Store fuel sources for VAPDIF

DDIAM Calculate rate of change in droplet diameter

DIFFUS Calculate mass diffusivity

DISTEM Determine distillation temperature

DRAGF Calculate droplet drag

DTEMP Calculate rate of change of droplet temperature

FBIN Calculate binomial distribution

FINTP Interpolate flow field of air

FNØZ Calculate initial conditions for droplets

FPRØP Determine fluid properties of film

GAMFUN Calculate Gamma function

GPRØP Determine gas properties for droplet

INPUT Read Input data

INTIAL Initialization of particle classes

LØCGRD Determine two largest classes

LØGCØL Logic for Droplet collision model

LØØK Interpolation for table lookup

NUSSET Calculate Nusselt number

ØUTPUT Write initial input conditions

PARPAT Integrate particle path equations

PFILM Calculate local film properties

PØLY Perform polynomial curve fit

PPRØP Determine fluid properties of droplets

PRINT Print class properties at each station

PTRAK Main program

SMTER Calculate summary terms

SUMRY Write summary output

TRACK Track droplet particle classes

VAHR Calculate heat and mass transfer rates

WALLRB Logic for wall rebounds

XRATE Calculate net production of X₂

XX2 Calculate X2 for one time step

X2INIT Initialize X2 mole concentration

X2MASS Calculate mass of X2 in droplet

8.4 List of COMMON BLOCK Variables

The COMMON BLOCK variables are grouped into labeled COMMON BLOCKS. Alphabetical listing is by labeled COMMON BLOCK name. The COMMON BLOCK name is given and a general description of the variables in the group. Following this is a detailed list of variables in the order in which they appear in the COMMON BLOCK. COMMON BLOCK variables for the ADD code are given in Ref. 4.

CØMMØN/ACØNS/	ADD Co	de Variables (Ref. 4)
COMMON/APART/		Droplet Input Conditions
RNZCLI(N,1)	r	Injector radius (cm)
RNZCLI(N,2)	z	Injector axial location (cm)
RNZCLI(N,3)	ф	Injector circumferential location (rad.)
RNZI(N)		Radial displacement of r (cm)
ALPHI(N)	α	Angle between normal and streamwise (deg)
BETAI(N)	β	Angle between tangential and streamwise (deg)
VMEANI(N)	v	Magnitude of velocity (M/sec)
DPRTI(N)	$\mathtt{D}_{\mathtt{L}}$	Mean diameter of droplet (micron)
DDPRTI(N)	$\delta D_{\boldsymbol{L}}$	Variance of droplet diameter (micron)
NNØZ		Number of ejectors
DALP(N)	δα	Variance in a (deg)
DBET(N)	δβ	Variance in β (deg)
ILØC		Number of ejectors
IVS		Number of velocity classes
IPHI		Number of a classes
ITHE		Number of β classes
IDIA		Number of droplet diameter classes
DVMI (N)	δV	Variance of Mean Velocity

COMMON/BONVAR/		Crossection Boundary Variables
C1,C2		Wall rebound probability constants
RTIP	r _H	Tip radius (cm)
RHVB	r _T	Hub radius (cm)
LPHI		Number of ϕ grid point
DPH1	Δφ	Increment in ϕ (rad)
LPART		Index in ϕ
PHIL	ΦL	Left \$\phi\$ boundary (rad)
PHIR	φ _r	Right \(\phi \) boundary (rad)
RPART(L,1)	r _t (ϕ)	Tip boundary (cm)
RPART (1,2)	r _H (φ)	Hup boundary (cm)
PHPART (K,1)	φ _L (r)	Left & boundary (rad)
PHPART (K,2)	φ _r (r)	Right & boundary (rad)
COMMON/BPART/	Droplet I	nput Thermodynamic Properties
RHØLPI(I)	ρL	Droplet density (gm/cm ³)
TEMPI(I)	$\mathtt{T_L}$	Droplet temperature (*K)
DLP(I)	$\mathbf{D}_{\mathbf{L}}$	Droplet diameter (micron)
KPART(N)		Radial index for Nth droplet
PERLØC(I)	P_{L}	Percentage of fuel
JPLL		

COMMON/CARRAY/	Thermody	namic Polynomial Coeff.
CØEFP(1,I)	AI	Droplet density (gm/cm ³)
CØEFT(2,1)	AI	Droplet heat capacity (cal/cm/°K/sec)
COEFP(3,1)	AI	Droplet viscosity (gm/cm/sec)
CØEFP(4,I)	AI	Gas heat capacity (cal/gm/°K)
COEFP(5,I)	AI	Gas conductivity (cal/cm/°K/sec)
CØEFP(6,1)	AI	Gas Viscosity (gm/cm/sec)
CØEFP(7,1)	AI	Air heat capacity (cal/gm/°K)
COEFP(8,I)	AI	Air conductivity (cal/cm/*K/sec)
CØEFP (9,1)	AI	Air viscosity (gm/cm/sec)
$F(T) = \sum_{i=1}^{n} x_i^2$	A _I T ^{I-}	1
I	•1	

COMMON CCRATE	Parameters for Critical Spacies	
AB, AF	A_b , A_f	
EB, EF	E _b , E _f	
ALPB, ALPF	A_b , A_f E_b , E_f a_b , a_f Constants in rate equation	
BETB, BETF	β_b , β_f γ_B , γ_B (Eq. 8.3.1)	
GAMB, GAMF	$\gamma_{\mathbf{B}}, \gamma_{\mathbf{B}}$	
CARBN	δ /	
MOLE1,MØLE2	M ₁ ,M ₂ Molecular weights	
BRAD	(r _d +b)/r _d Film thickness ratio	
YO2	Y _{O2} Mole fraction of O ₂	
DELM2	$(x_2/x_1)_o$ Initial ratio	
LRLP	Number of points in film	

DELTB, DELTF Constants for rate equation ANUB, ANUF (Eq. 8.3.11) COMMON /CCX21/ Mole Concentration Critical Species X21 X₂(t) Mole concentration (mole/cm³) Mole concentration (mole/cm³) $X_2(t+\Delta t)$ X22(I) $(dX_2/dt)_{t+\Lambda}$ Production of X₂ (mole/cm³/sec) DX2DO(1) Production of X₂ (mole/cm³/sec) $(dX_2/dt)_{+}$ DX2DT(I) COMMON /COLLVA/ Index for Largest Class KGEØM(K,L,1)Index for large t class KGEØM(K,L,2)Index for second largest class Where K = r grid index L = \phi grid index COMMON /CØNST/ ADD Code (Ref. 4) COMMON /CONVER/ Constants Force equivalent of mass (1.01325x10⁶ dyn/cm/atm) GC g Energy equivalent of work (41.311cm³mole/atm/°K) **JCØNST** J Universal Gas Constant (82.087 cm³atm/mole/°K) RØCØN R Universal Gas Constant (1.98717 cal/mol/°K) RØCØNP CØMMØN /CORE/ ADD Code (Ref. 4) ADD Code (Ref. 4) /CORE2/ COMMON COMMON /COXCUR/ Cox chart data Number of input points ICØX1 PICH P_1 Vapor pressure (atm)

P2CH	P_2	Vapor pressure (atm)
CØXCAR(1,1)	n	Carbon number
CØXCAR(2,I)	т ₁	(Τ(ζ,P ₁) (°K)
CØXCAR(3,I)	т ₂	$T(\zeta,P_2)$ (°K)
CØMMØN /CPART/	Dependent drop	olet variables
PART(1,1)	v_s	Streamwise velocity (m/sec)
PART(I,2)	U _¢	Tangential velocity (m/sec)
PART(1,3)	$\mathbf{u}_{\mathbf{n}}$	Normal velocity (m/sec)
PART(1,4)	n	Normal coordinate
PART(I,5)	ф	Circumferential coordinate
PART(I,6)	$^{\mathrm{D}}\mathrm{_{L}}$	Droplet diameter (micron)
PART(I,7)	$^{\mathrm{T}}_{\mathrm{L}}$	Droplet temperature (°K)
PART(1,8)	r	Droplet radius (cm)
PART(1,9)	z	Droplet axial distance (cm)
PART(1,10)	t	Droplet time (sec)
PART(1,11)	f	Probability
PART(1,12)	M_2	Mass of critical species (gm)
PART(1,13)	Q	Total heat load (cal)
COMMON /CURVE/ I	Distilation cur	rve
IDSTIL		No. of data points
DISCUR(1,1)	$P_{\mathbf{e}}$	Percent evaporated
DISCUR(2,1)	T_{b}	Temperature (°K)

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CØMMØN /DRED1/ A	DD code (Ref.	4)
cømmøn /dskløc/	ADD code (Ref.	4)
COMMON /DUCOUT/	ADD code (Ref.	4)
COMMON /DUCTIN/	ADD code (Rei	:. 4)
COMMON /FILVAR/	Film thermody	namic properties
MF	M _m	Film molecular weight
RHØF	$\rho_{\mathbf{m}}$	Film density (gm/cm ³)
CPF	C _{pm}	Film heat capacity (cal/gm/°K)
KF	k m	Film thermal conductivity (cal/cm/°K/sec)
MUF	μ _m	Film viscosity (gm/cm/sec)
DMASSF	m	Film mass diffusivity (cm ² /sec)
CFF	c _f	Fuel mass fraction
CGF	C _a	Air mass fraction
SIGP6F	$\sigma_{f m}$	Film force constant (A)
OMEGF	\mathfrak{Q}_{igstar}	Collision integral
YINF	Y_{∞}	Air mole fraction
YGF	1-Y _m	Average film air mole fraction
YPF	Y _m	Average film fuel mole fraction
YPSF	Y _{f,s}	Fuel mole fraction at droplet surface
CKPGF	(ε/κ) _m	Force constant film (°K)
TSTARF	т*	Dimensionless temperature
YPINF	Y _{f,∞}	Mole fraction of air at film edge
MINF	Ma	Molecular weight air

COMMON	/FLAGS/	ADD code	(Ref.	4)
COMMON	/FUNC/	ADD code	(Ref.	4)
CØMMØN	/GASVAR/	Gas therm	odynam	mic properties
MG		Ma		Air molecular weight
PCG		Pca		Air critical pressure (atm)
TCG		T _{ca}		Air critical temperature (°K)
SIGG		$G_{\mathbf{a}}$		Air force constant (Å)
CKG		(ε/κ) _a		Air force constant (°K)
CPG		C _{pa}		Air heat capacity (cal/gm/°K)
KG		k a		Air thermal conductivity (cal/cm/°K/sec)
MUG		$^{\mu}$ a	1	Air viscosity (gm/cm/sec)
COMMON	/INTINP/			Input Flags
KL				No. of streamlines
JL				No. of streamwise stations
KDS				No. steps/course grid
KLL				Not used
NB				Not used
ISHAPE				Not used
IØPTN				Input option see Section 5.2
N = 1,1	7			
CØMMØN	/MASSD/	Source t	erms f	for VAPDIF code
AMASS(K		° w _f ,S _d ,∆T		Source terms for VAPDIF
RDUM(K,		o w fw		Wall source terms for VAPDIF

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APARM(1)	Δφ ,	Circumferential step size (rad)
APARM(2)	LPHT ,	No. circumferential steps
APARM(3)	W _{fv} ,	Weight flow fuel (gm/sec)
APARM(4)	W _{fa} ,	Weight flow air. (gm/sec)
APARM(5)	JLAST ,	Number of blocks
APARM(6)	ΙφΡΤ3 ,	input option
APARM(7)	JCφUN ,	Block routine
COMMON /MISCEL/	Miscellaneo	us variahles
VEL	v	Air velocity (m/sec)
TEMG	T _a	Air temperature (°K)
PRESG	P _a	Air pressure (atm)
RHØG	P _a	Air density (gm/cm ³)
COMMON /NUMDEN/	Droplet Sum	mary
FMASS	$\overset{\mathtt{o}}{\mathtt{w}}_{\mathtt{L}}$	Fuel flow rate (gm/sec)
FSUM	N _T	No. fuel droplets/sec (1/sec)
SMDD		SMD denominator
SMDN		SMD numerator
SMD	SMD	Sauter mean diameter (microns)
QF	$\mathring{\mathtt{w}}_{\mathtt{L}}$	Liquid fuel flow rate (gm/sec)
QFO	w W	Initial liquid fuel flow rate (gm/sec)
	w _{LO}	
SARRAY(1)	LO z	Axial location (cm)
SARRAY(1) SARRAY(2)		

R8	2-	0	1 5	2	۷	2	_/.	n
KO.	4-	3	IJ		o	4	-•	u

SARRAY(4)		% fuel at wall that is liquid
SARRAY(5)		% fuel at wall that is vapor
SARRAY(6)		% fuel in vapor state
SARRAY(7)		% fuel evaporated
SARRAY(8)		Flow rate of vaporized fuel
SARRAY(9)		Fuel/Air ratio
COMMON /NUSVAR/	Nusselt numb	oer variables
NUH	Nu _h	Nusselt number heat transfer
NUM	Nu _m	Nusselt number mass transfer
REN	Re _D	Reynolds number of droplet
PRN	Pr	Prandtle number
SCN	Sc	Schmidt number
COMMON / PARVAR/	Droplet therm	modynamic properties
MP	M _L	Molecular weight fuel
TCP .	T _c	Critical temperature of fuel (°K)
PCP	P _c	Critical pressure of fuel (atm)
SIGP	σL	Force constant (Å)
СКР	(ε/κ) _L	Force constant (°K)
LAMBP	$^{\lambda}{}_{\mathbf{L}}$	Heat of vaporization (cal/gm)
SP	S	Surface tension (dyne/cm)
PVP	P _{f,s}	Vapor pressure fuel (atm)
TMP	T _m	Film temperature (°K)
RHØLP	$^{ ho}$ L	Fuel liquid density (gm/cm ³)
CPLP	$c_{_{\mathrm{PL}}}$	Fuel liquid heat capacity (cal/gm/°K)

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MULP	μ _L Fuel	liquid viscosity (gm/cm/sec)
CPVP	C Fuel	vapor heat capacity (cal/gm/°K)
KVP	k Fuel	vapor thermal conductivity (cal/cm/°K/sec)
MUVP	μ Fuel	vapor viscosity (gm/cm/sec)
cømmøn /qmøn/		
QØLD(I)	q Heat	transfer rate (cal/sec)
DMDTO(I)	(dm2/dt) Mass	rate of change of critical species
CØMMØN /REALIN/	ADD code (Ref. 4)	
CØMMØN /SVARB/	ADD code (Ref. 4)	

8.5 List of Local Variables

A list of selected local variables appears below. These variables are alphabetically listed by subroutine name.

AL	J	P	Ø	Т	•
-	-	_	-	_	-

TS T* , Dimensionless temperature

ALJP \emptyset T Ω^* , Collision integral

BLKDAT ADD code (Ref. 4)

BLKRED ADD code (Ref. 4)

BØUNCE

IJK Class index

IBØUN Wall index

SP Surface tension (dyne/cm)

TEMMIN Minimum droplet temperature (°K)

TEMMAX Maximum droplet temperature (°K)

ND N_{T} Number of droplets (1/sec)

PRB Probability of wall rebound

WFCØLL Amount of fuel/area (gm/cm²)

WFEVDP Amount of fuel evaporated/area (gm/cm²)

WFEVAT Total fuel evaporated (gm)

WFLIQT Total fuel on wall (gm)

BREKUP

IJK Droplet class index

IPREK Flag indicates shattering

A,B Constant Wolfe, Anderson shattering model

AK1, AK2 Aerodynamic drag constants

CD	c _D	Drag coefficient CD+1
DK3		Shattering Model constants DK3=136
FK1,FK2		Friction drag constants FK1=2, FK2=4
RHØLP	$^{ m ho}_{ m L}$	Density of droplet (gm/cm ³)
SP	S	Surface tension (dyn/cm)
VEL	V	Absolute velocity (m/sec)
DSHAT		Droplet diameter after shattering (micron)
ND	N _T	Total number density after shattering (1/sec)
TEST1		Time of aerodynamic breakup (sec)
TEST2		Time of friction breakup (sec)
CØLDYN		
IP1,IP2		Index for colliding classes
VEL11, VEL12, VEL1	3 \vec{v}_J	Velocity after collision (Vs, $Vn,V\phi$) (m/sec)
VEL21, VEL22, V23	$\overline{v}_{\mathbf{k}}$	Velocity after collision (Vs,Vn,V¢) (m/sec)
AMASS1,AMASS2	m _J ,m _K	Droplet mass before collision (gm)
E,EI	E,E ⁻¹	Velocity transformation matrix
VCØL1,VCØL2	\vec{v}_{J},\vec{v}_{K}	Velocity in collision coordinates (m/sec)
UC1,UC2	V _{CJ1} ,V _{CK1}	Velocity before collision (m/sec)
VCL,VC2	V _{CJ2} ,V _{CK2}	Velocity after collision (m/sec)
CØLLDE		
K,J		Droplet index
RC	R _C	Distance between droplets (cm)
XC,YC,ZC	x _c ,y _c ,z _c	Relative coordinates (cm)

COLLSN

IP1,IP2		Droplet index
XC,YC,Zc	X_{c}, Y_{c}, Z_{c}	Relative cartesian coordinates (cm)
A(1,J)		Transform matrix streamline to cylindrical
B(I,J)		Transform matrix cylindrical to cartesian
C(1,J)		Transform matrix streamline to cartesian
D(I,J)		Transform matrix cartesian to droplet
E(I,J)	E	Transform matrix streamline to droplet
EI(1,J)	E ⁻¹	Transform matrix droplet to streamline
CØØR	ADD code (Ref	. 4)
СФХСНТ		
PRESS	Pv	Vapor pressure (atm)
BCØEF	$^{\beta}$ n	Cox chart constants
TEM1	T _L	Droplet temperature
PERCT	Pc	Percent evaporated
DATAM		
ΙØΡ		Module switch
JCØUN		Block counter
DDIAM		
WDØTSF	w _I .	Vaporization rate (gm/sec)
DRDT	d(p _L)/dt	Rate of density change (gm/cm ³ /sec)
DLP	D _{I.}	Droplet diameter (micron)
DDIAM	d(D ₁)/dt	Rate of diameter change (micron/sec)

Section 2

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DIFFUS		
TEMP	T	Temperature (°K)
PINF	P _a	Air pressure (atm)
DIFFUS		Mass diffusion coefficient (cm ² /sec)
DISTEM		
PER	P _e	Percent liquid evaporated
DISTEM	T _D	Distallation temperature
DRAGF		
RHØ	$^{ m ho}_{ m L}$	Droplet density (gm/cm ³)
DLP	$^{\mathtt{D}}_{\mathtt{L}}$	Droplet diameter (micron)
TINF	Ta	Air temperature (°K)
PINF	P _a	Air pressure (atm)
VINF	v	Air velocity (m/sec)
VPART	$v_{\mathtt{i}}$	Droplet velocity (m/sec)
VEL	ΔV	Relative velocity (m/sec)
CD	C _D	Drag coefficient
DTEMP		
QNET	$\mathbf{q}_{\mathbf{s}} - \mathbf{w}_{\mathbf{L}}^{\lambda}$	Net heat flux (cal/sec)
DLP	$^{\mathrm{D}}_{\mathrm{L}}$	Droplet diameter (micron)
DTEMP	dT/dt	Rate of temperature change (°K/sec)
FBIN		
IXX		IXX th class
JXX		Total number of classes
FBIN	f(I,IL)	Probability

FINTP		
ANE	n	Normal coordinate
vv		Metric coefficient
VS,VP	v_{s}, v_{ϕ}	Air velocity components (m/sec)
RØ	$^{ ho}{f a}$	Air density (gm/cm ³)
TP	T _a	Air temperature (°K)
PS	Pa	Air pressure (atm)
RB,ZB	r,z	Coordinates of droplet (cm)
RSB,RNB		Direction cosines of coordinates
VSB, VNB		Curvatures of coordinates
KP		Streamline index for droplet
M		Index for solution variables
FNØZ		
ANP	n	Normal coordinate
HEIT	н	Duct height (cm)
FL, FV, FT, FP, FD	f _L , f _v , f _t , f _p , f _o	Probability functions
PÊ	ф	Circumferential location (rad)
RP,ZP	r,z	Droplet coordinates (cm)
VSP, VNP, VPP	v _s ,v _n ,v _p	Droplet velocity (m/sec)
FPRØP		Mar (ata)
PINP	Pa	Air pressure (atm)
GAMFUN ARG	x	Argument
GAMFUN	Γ (X)	Gamma Function

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GPRØP		
CPG	C _{pa}	Air heat capacity (cal/gm/*K)
KG	k _a	Air thermal conductivity (cal/cm/°K/sec)
MUG	μ a	Air viscosity (gm/cm/sec)
INPUT See Sect	ion 5.2	
INTIAL See COM	MON BLOCK varia	ables
LOCGRD I.JK		Index for iroplet class
LØGCØL		
X1,Y1,Z1	x_{J}, y_{J}, z_{J}	Cartesian coordinates J th droplet (cm)
X2,Y2,Z2	x _K ,y _K ,z _C	Cartesian coordinates K th droplet (cm)
XC,YC,ZC	x _c ,y _c ,z _c	Relative cartesian coordinates (cm)
RC	R _C	Distance along line of center (cm)
LØØK		
X(I)	x _I	Table of abscissa values
Y(I)	YI	Table of ordinate values
XIN	x	Input abscissa
YØUT	Y	Output ordinate
кк		Default flag
NUSSET See COM	MØN /NUSVAR/	
ØUTPUT Self ex	cplanatory	
PARPAT		
VS1,VN1,VP1	V _s ,V _n ,V _φ	Droplet velocity components at t (m/sec)
AN1	n	Normal coordinate at t
P1	ф	Circumferential location at t (rad)
DLP1	D _L	Droplet diameter at t (micron)

TLP1	T _L	Droplet temperature at t (°K)
VS2,VN2,YP2	V V V s n ¢	Droplet velocity components t+dt (m/sec)
AN2	n	Normal coordinate at t+dt
P2	ф	Circumferential location t+dt (rad)
DLP2	$^{\mathrm{D}}\mathrm{_{L}}$	Droplet diameter at t+dt (micron)
TLP2	T _L	Droplet temperature at t+dt (°K)
RB2,ZB2	r,z	Droplet coordinates at t+dt (cm)
RHØLPO	ρLO	Initial droplet density (gm/cm ³)
DLPO	DLO	Initial droplet diameter (micron)
KP	KP	Streamline index
DT2	Δt	Time increment
QS1	q	Droplet heat transfer rate at t (cal/sec)
X2M2	^m 2	Mass of critical species at t+dt (gm)
QHEAT1	Q_{1}	Total heat added to droplet at t (cal
QHEAT2	Q_2	Total heat added to droplet at t+dt (cal)
DM1	d(m2)/dt	Rate of change of mass at t (gm/sec)
PFILM		
RL	r ^r +p	Droplet film radius (micron)
RLP	r _L	Droplet radius (micron)
TLP	T _L	Droplet temperature (°K)
PINF	P _a	Air pressure (atm)
PF	P _f	Vapor pressure fuel (atm)
TF	' _f	Temperature of fuel (°K)
XF	$\mathbf{x}_{\mathbf{f}}$	Mole concentration of fuel (mole/cm ³)

FØLY

1		Property index
TEM	т	Temperature *K
PPRØP		
TINF	T _a	Air temperature (°K)
TLP	T _L	Droplet temperature (°K)
DLP	D _L	Droplet diameter (micron)
RHØLPO	° LO	Initial droplet density (gm/cm ³)
DPLO	D _{LO}	Initial droplet diameter (micron)
PRINT	Self explana	tory
PTRAK		
FMC		Conversion factor (cm/ft)
RHUB, ZHUB	r _H ,z _H	ID wall coordinates (cm)
RT1P,ZTIP	$\mathbf{r}_{\mathbf{T}}$, $\mathbf{z}_{\mathbf{T}}$	OD wall coordinates (cm)
SMTER		
WAIR	w _u	Weight flow air (gm/sec)
WFEVAT		Weight flow gas (gm/sec)
WFLIQT	. W _{1.}	Weight flow liquid droplets (gm/sec)
QF	w _{LO}	Initial fuel flow (gm/sec)
z	z	Axial location (cm)
SUMRY Self expl	anatory	

TRACK	
	~

IDIA No. diameter classes

ILØC No. location classes

IPHI No. normal angle classes

ITHE No. asmutial angle classes

IVS No. velocity classes

IJK Class index

VAHR

QNET $q - w \lambda$ Net heat transfer rate (cal/sec)

WDØTSF w. Vaporization rate (gm/sec)

TLP T_L Droplet temperature (°K)

DLP D Droplet diameter (micron)

TINF T_a Air temperature (°K)

PINF P_a Air pressure (atm)

WALLRB

IJK Droplet class index

XRATE

T Temperature (°K)

 X_1 Mole concentration species 1 (mole/cm³)

 X_2 Mole concentration species 2 (mole/cm³)

 x_{02} Mole concentration oxygen (mole/cm³)

<u>xx2</u>		
DLP1	D_{L}	Droplet diameter at t (microns)
DT2	Δt	Time step (sec)
TLP	T _L	Droplet temperature (°K)
PINF	P _a	Air pressure (atm)
TINF	T _a	Air temperature (°K)
X2INIT		
DLP	D_{L}	Droplet diameter (micron)
TLP	T _L	Droplet temperature (°K)
PINF	P _a	Air pressure (atm)
TINF	T _a	Air temperature (°K)
X2M2	M ₂	Mass critical species (gm)
QIT Ø T	$Q_{\mathbf{L}}$	Total heat added to droplet (cal)
X2MASS		
BRAD	(r _d +b)/r _d	Film thickness ratio
DLP1, DLP2	$^{\mathrm{D}}_{\mathrm{L}}$	Droplet diameter at t Rt+dt (micron)
Dn2DT	dM ₂ /dt	Rate of mass change critical species (gm/sec)

Time step sec

dt

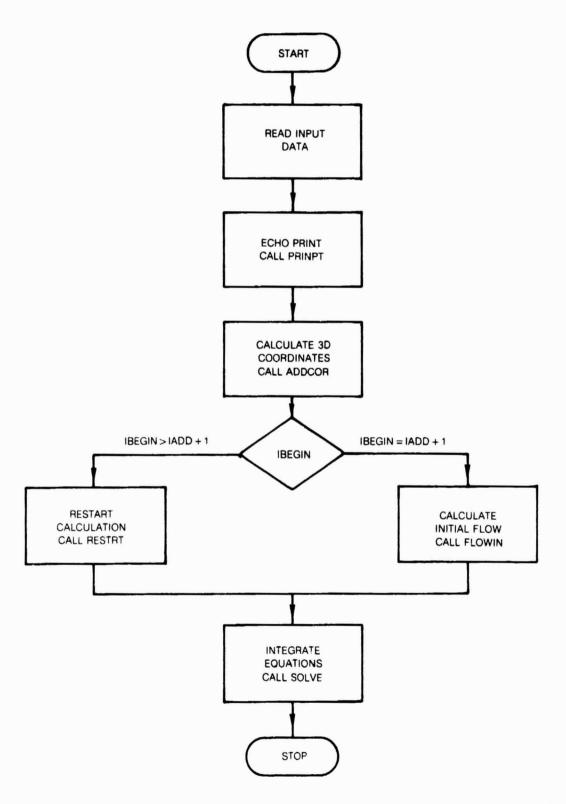
DT2

9.0 DETAIL DESCRIPTION OF VAPDIF CODE

9.1 Main Program/Flow Chart

The flow chart for the main program for the VAPDIF code is shown on Fig. 9.1. It consists of four major tasks: 1) Read and print the input data; 2) Calculate the three dimensional coordinates; 3) Calculate or restart initial conditions; and 4) Solve the diffusion equation. The run stream for execution of the code is given in Section 6.1. This run stream includes both input and output data files. A table of output file assignments is given on Table 7.3 and a table of unit numbers is given by Table 9.1. Table 9.1 shows both input and output files. NOP is the unit index used by the I/O routines. For input files the code generating the data is given by the code name in brackets. For output files the subroutine generating the data is given without brackets.

FLOW CHART FOR MAIN PROGRAM FOR VAPDIF



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9.2 Description of Modules by Major Task

A complete list and brief description of all the subroutines is given in Section 9.3. The flow chart for the main program for VAPDIF is shown in Fig. 9.1 with an overall description given in Section 9.1. The description of the module functions will follow this flow chart. Only major tasks will be described. Input/Output routines are self explanatory and will not be described. Of the task shown on Fig. 9.1 only tasks two and four need be described.

Subroutine ADDCØR generates the three dimensional coordinate system used by the VAPDIF. Coordinates generated by the ADD code and stored on file 9, are read block by block. Each block corresponds to on streamwise station. ADDCØR then calculates the coordinates, metrics, and arc length distance and stores the result on unit 10. It then calculates the three dimensional cartesian coordinates for each mesh point and stores the results on unit 12. Finally it calculates the transformation matrix from the computational coordinates to the cartesian coordinates and stores the result on unit 13. Data on units 12 and 13 are not necessary for the solution but are useful for plotting results in physical space.

Subroutine SØLVE solves the diffusion equation (Eq. 5.2.1) or the critical species equation (Eq. 8.2.1) depending on the input option ISDG. The main program sets the first and last station. A flow chart for subroutine SØLVE is shown on Fig. 9.2. The first task is to align the data blocks on units 8, 17 and 28 with the absolute coordinate location of the coordinate grid stored on unit 9. The I DØ loop steps off streamwise stations from ILOW to INUM. Next flow field data calculated by the ADD code and stored on unit 8 is read and source terms stored on units 17 and 28 are read. The V DØ loop is an iteration loop for the point relaxation algorithm described in Section 5.1, and the K and J DØ loops sweep the entire crossplane grid including the boundary points. The coordinates stored on unit 10 are read by RDINB. The coefficients of the differential equations are calculated by CØEFFI. For ISDG>0 CØEFSG calculates the source term S_{ρ} for the critical species equation (Eq. 8.2.1). On the boundaries, PBNDC applies normal derivative boundary conditions, and PERBC applies periodic boundary conditions depending on the input options. PØISSN applies the difference operators (see Section 5.1) and solves for the Vth guess. With the completion of J, K grid sweep, a convergence check is made. If the solution converges, the solution is printed by PRTDSK and stores on unit 11 by WRØUT. The calculation then moves to the next station until the I DØ loop is completed. The calculation then returns to the main program.

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FLOW CHART FOR SUBROUTINE SOLVE

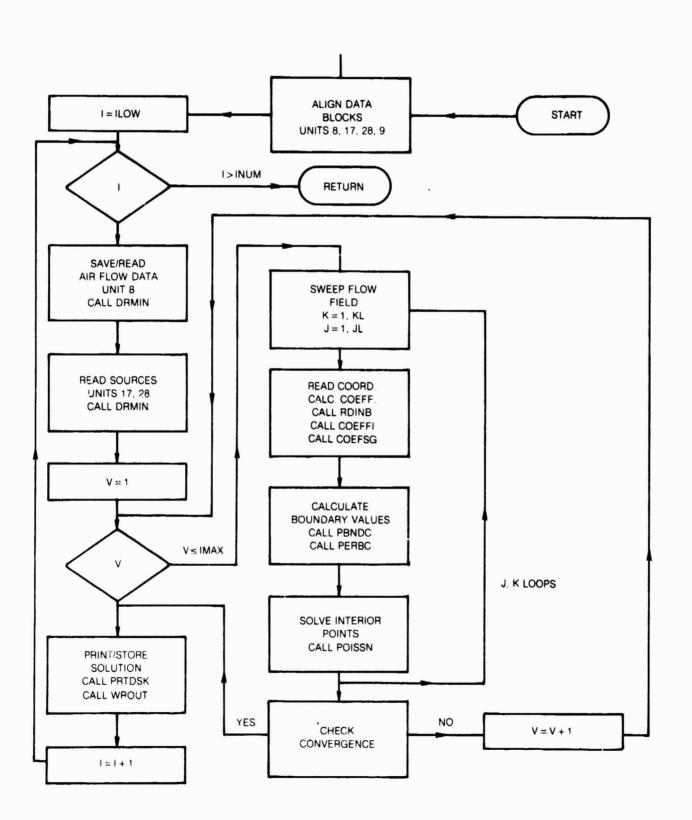


Table 9.1

Table of Unit Numbers

N Ø P	NAME	UNIT	SUBROUTINE (CODE)	DATA
1	IYDRM	10	ADDCØR	3D coordinates
2	IFDRM	11	SØLVE	Output file
3	IXDRM	12	ADDCØR	3D Castesian coordinates
4	ITDRM	13	ADDCØR	3D transformation matrix
5	INDRM	17	(VAPDIF)	Mass fraction of fuel
6	IADDRM	8	(ADD)	Air flow field
7	ICØDRM	9	(ADD)	Axisymmetric coordinates
8	IFGDRM	19	(PTRAK)	Summary droplet data
9	28	28	(PTlack)	Critical species source

9.3 List of Subroutines in VAPDIF

ADDCØR Calculate 3D coordinates

AINTG Area integral of prescribed function

CØEFFI Calculate coefficients of P.D.E.

CØEFSG Calculate source for critical species

DERBDY Calculate derivatives on boundaries

DERINT Calculate interior derivatives

DERIV Calculate derivatives

DFCØR Correct fuel concentrate

DIFFUSE Main program

DM2DT Critical species rate equation

DRØUT Input/Output module

FLØWIN Initial conditions module

PBNDC Neuman boundary conditions

PERBC Periodic boundary conditions

PERIOD Read boundary values

PØISSN Solve Poisson's equation

PRINPT Print module

PRUN Metric conversion

PRTDSK Print module

RDINA Read contiguous block data

RDINB Read overlapping block data

RESTRT Restart module

RHØV Integrand for flow integration

SØLVE PDE solution algorithm

SØURCE Integrand for area integral

SUMRY Print summary data

WRØUT Write contiguous block data

WRØUTB Write overlapping block data

WTFLØW Integrand of Mass flow area integral

9.4 List of COMMON BLOCK Variables

The CØMMØN BLOCK variables are grouped into labeled CØMMØN BLØCKS. Alphabetical listing is by labeled CØMMØN BLØCK name. The CØMMØN BLØCK name is given and a general description of the variables in the group. Following this is a detailed list of variables in the order in which they appear in the CØMMØN BLØCK. CØMMØN BLØCK variables for the ADD code are given in Ref. 4.

CØMMØN /CADD/ ADD code Air flow variables (Ref. 4)

COMMON /CCRATE/	Variables for	critical species rate equation
ISDG		Option flag
SDG	S _g	Source of critical species
AB, AF	A _b , A _f	
EB, EF	E _b ,E _f	Constants in Eq. 8.3.1
ALPB, ALPF	a _b ,a _f	
BETB, BETF	β _b ,β _f	
GAMB, GAMF	γ _b ,γ _f	
CARBN	ζ	Carbon number
RØCØNP	R	Gas constant (1.98717 cal/mole/°K)
MØLE1,MØLE2	$^{\mathrm{M}}_{1}, ^{\mathrm{M}}_{2}$	Molecular weights
Y02	Y ₀₂	Mole fraction of 0_2
DELTB, DELTF	δ _b ,δ _f	Constants in Eq. 8.3.11
ANUB, ANUF	^δ b, δf ν _b , ν _f	constants in Eq. 6.5.11
ISGMAX		Flag
CØMMØN /CF/ Dependent Variable		
F(J,K)	f ^{I-1} J,K	Dependent variable at I-1, J,K

COMMON /CFF/ Coefficient of PDE		
A2(J),A3(J) A ₂ ,A ₃	Coefficient of second derivative	
B2(J), B3(J) B ₃ ,B ₃	Coefficient of first derivative	
C(J) C	Coefficient of function	
COMMON /CFG/ Dependent Varia	ble	
$GF(J,K)$ $f_{J,K}^{I}$	Dependent variable at I,J,K	
COMMON /CFG2/ Mass fraction	fuel	
$FG2(J,K)$ $C_{J,K}^{I}$	Mass fraction of fuel	
COMMON /CMU/ Turbulent visco	sity	
XMUT(J) μ _Γ	Turbulent viscosity (gm/cm/sec)	
COMMON /CONV/ Conversion fac	tors	
FTCM	30.48 cm/ft	
LBKG	.4538 lb/kg	
CKELRK	1.8 °R/°K	
FTM	.3048 m/ft	
COMMON /CT/ Coordinate trans	formation matrix	
$TCØR(L,M,J,K)$ $T_{I,J,K}^{L,M}$	Coordinate rotation matrix at I,J,K	
COMMON /CX/ Cartesian coordinates		
$X(L,J,K)$ X_L	Cartesian coordinate of point I,J,K	
COMMON /CY/ Computational coordinates at I		
Y(L,M,J,K)		
L = 1	Streamwise direction	
= 2 = 3	Principal normal direction	
- 3	Orthogonal direction	

M = 1 = 2 = 3	Y h y	Coordinate at point I,J,K Metric (cm) Arc length (cm)
CØMMØN /CYI/ C	omputational co	ordinates at I-1
YI(L,M,J,K)		See CØMMØN /CY/
COMMON /DATABL/	I/O index da	ta (see Table 9.1)
INDX (NØP,1)		Unit number
INDX (NØP,2)		Block length
INDX (NØP,3)		Pointer location
INDX (NØP,4)		Not used
INDX (NØP,5)		NOT USED
COMMON /RESIDL/	Residuals	
RES		Residual
IMAX		Max no. iterations
EPSLØN		Tolerance
PCT		Percent change cutoff
RLX		Relaxation parameter
COMMON /SAVC/ Solution variable on periodic boundary		
C2(J)	C(J,1)	Fuel mass fraction K=1 boundary
CKLM1(J)	C(J,KL)	Fuel mass fraction K=1 boundary
C¢MMØN /SAVF/ Air flow variables		
FLØSAV(L,J)		See ADD code

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COMMON /SOURC/	Sources	for fuel concentration equation
W(J,K)	ů _L	Source terms (gm/cm ³ /sec)
BDYY(L,M,J)	w _{LW}	Wall source terms gm/cm ² /sec
WPARM(L)		See CØMMØN/MASSD/ in PTRAK
CØMMØN/SØURC2/	Sources	for critical species equation
W2(J,K)	s _d	Source for critical species equation

9.5 List of Local Variables

A list of selected local variables appears below. These variables are alphabetically listed by subroutine name.

ADDCØR (Ref. 4)		
Q(N,J)		ADD code variables
ILA		No. streamwise stations
JLA		No. normal stations
IL,JL,KL		No. mesh points in Y_1 , Y_2 , Y_3 directions
RADR	r r	Reference length
DSTEP	$\Delta \mathbf{s}$	Y ₁ step size
DPHI	$\Lambda \Phi$	Y ₃ step size
AINTG		
AINT		Area integral of f
1		Axial station
FCN	f	Integrand of integral
FUNCT		Dummy subroutine name
CØEFFI (Ref. ')		
F(INVAR,1,J)		Air flow variables from ADD code
SCHM	Se	Schmidt number
USR	u r	Reference velocity
RHØR	$^{ m p}$ r	Reference density
TEMPR	$\mathbf{r}_{\mathbf{r}}$	Reference temperature
VISCR	\mathbf{r}	Reference viscosity

PRFSR	P _r	Reference pressure
DSTEP	Δs	Y ₁ step size
CØEFSG		
RØCØN	R	Gas constant (82.0575 cm atm/mole/°K)
røcønp	R	Gas constant (1.9817 cal/mole/°K)
TINF	T _a	Air temperature (°K)
PJNF	P _a	Air pressure (atm)
UINF	U	Air velocity (m/sec)
X02	х ₀₂	Mole concentration of oxygen (mole/cm ³)
Y02	Y ₀₂	Mole fraction of oxygen
DERBDY		
ID		Direction index
IV		Variable index
ITYPE		Option
DIN	f	Input array (dependent variable)
11,12,13		Dimensions of DIN
YIN	Y	Input array (independent variable)
J0,K0		Smallest indices
DG	df/dy	First derivative
DDG	d ² f/dy ²	Second derivative
B,A		Intermediate values

DERINT

See subroutine DERBDY

DERIV

See subroutine DERBDY

DFCØR

WRATIO Fuel mass flow correction factor

BIFFUS

IADD Add code strating station

IBEGIN Starting station

IEND Ending station

DM2DT See CØMMØN/CCRATE/

DRØUT

INUNIT Unit number

ADDR Output address

BLØCK Record length (words)

NMØVE Relative address

FLØWIN

CONC C Initial mass fraction of fuel

PBNDC

AC, BC, CC, DC Coefficient PDE

BDYVAL Boundary value

J,K Mesh point

JJ,KK Sub block mesh point

JBDY Boundary index

SØLN Solution

PERBC

See subroutine PBNDC

PØISSN

AC, BC, CC, DC

Coefficients of PDE

JJ, KK

Sub block mesh point

SØLN

Solution

PRINPT

See output format statements

PRRUN

See COMMON/CONV/

PRTDSK

IDX1, IDX2

Indices of variables

ISTAT

Unit index

NØP

Option

RDINA

I,J,K

Mesh point index

JJ,KK

Sub wock index

ADDR1

Block length

NØP

See Table 9.1

RDINB

See subroutine RDINA

RESTRT

IBEGIN

Starting station no.

PHØV

RH

ρu

Mass flux (slug/ft²/sec) /

RLXCAL

RLXCAL

Relaxation parameter (Eq. 5.3.14)

SØLVE

IADD ADD code station

IBEGIN, IEND Beginning/Ending station

J,K Mesh point

JJ,KK Sub block mesh point

ISIDE Boundary index

FTIL f^{v+1} Guess of solution

RES Residual

SØURCE

S w Integrand

SUMRY See output format statements

WRØUT See subroutine RDINA

WRØUTB See subroutine RDINA

WTFLØW

WF cou Mass flux fuel (slug/ft²/sec)

10.0 REFERENCES

- Anderson, O.L.: Finite Difference Solution for Turbulent Swirling Compressible Flow in Axisymmetric Ducts with Struts. NASA CR 2365 Feb. 1974.
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- Anderson, O.L. and D.E. Edwards: Extensions to an Analysis of Turbulent Swirling Compressible Flow in Axisymmetric Ducts NASA contract NAS3-21853, UTRC Report R81-914720-18. February 1981.
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